

Fatty acid and Lipid reference spectra

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The number of publications reporting lipid and fatty acid time-of-flight secondary ion mass spectrometry analysis has increased as ToF-SIMS is increasingly applied towards analysis of biological systems. Tissue and cell analysis through ToF-SIMS typically involves collecting mass spectrometry images that are used to characterize the local distribution of lipids and fatty acids throughout the analyzed area. Complete and reliable sets of reference spectra are required for fatty acids and lipids in order to aid in the interpretation of ToF-SIMS data from tissues and cells. Here, we present the reference spectra for 8 fatty acids and 1 lipid. This database contains positive and negative polarity spectra using a Bi³⁺ primary ion species.

Keywords: ToF-SIMS, fatty acids, standards

INTRODUCTION

No current database of fatty acids and lipids exists for ToF-SIMS. ToF-SIMS is a hard ionization technique and produces fragmentation patterns that are poorly understood, particularly in the case of tissue and cell analysis. Assignment of a chemical structure for a given peak is often vague for charged molecular ions, and/or their fragments¹. Here, we provide ToF-SIMS data from standards of 1 lipid and 8 fatty acids, as well as the corresponding peak lists of their fragmentation products.

All fatty acids with purities $\geq 99\%$ were purchased through Sigma Aldrich. Fatty acids in solid form were dissolved in ethanol (Sigma Aldrich) at a concentration of 5mg/mL. Fatty acids in liquid form were used without alterations. Host silicon wafers of 1×1 cm size were cleaned by soaking in ultrapure (18.2 M Ω) water overnight, rinsed, and then sonicated for two 5 minute cycles in dichloromethane, acetone, and methanol. 20 μ L of each fatty acid, either in solution or in liquid form, was then deposited onto separate silicon wafers using a digital pipette making sure that each deposited droplet was spread over the entire wafer surface. Samples were then vacuum dried at 226 mbar at room temperature in a clean vacuum oven.

The spectra were obtained on an IONTOF TOF.SIMS 5 equipped with a 25 keV bismuth metal ion gun. The instrument was operated in high current bunched mode. The primary ion dose was kept below the static limit (10¹² ions/cm²). The raster size was 500 × 500 μ m² with a raster resolution of 128 x 128 pixels, a cycle time of 100 μ s, and a primary ion current of 0.30 pA. 50 scans were acquired per single mass spectrum. Note that variations in mass resolution among the reference spectra are due to crystallization differences between the fatty acids resulting in changes in topography.

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Accession #s: 01488, 01489, 01490, 01491, 01492, 01493, 01494, 01495, 01496

Technique: SIMS

Host Material: Silicon (100) wafer

Instrument: IONTOF, TOF.SIMS 5

Major Species in Spectra: C, H, O, N

Minor Species in Spectra: Si, Cl

Published Spectra: 18

Spectra in Electronic Record: 54

Published Spectral Figures: 19

Spectral Category: Reference

Figures and tables presented contain the most prominent peaks. The major negative and positive secondary ion fragmentation products are presented next to their respective spectra. A full combined peak list for the major peaks present in the database for negative and positive secondary ions is shown in the spectral features tables, and the corresponding M - H and/or any M + H peaks for each of the samples are shown in Figure 1.

In the figures, the full molecule is referred to with "M." In the label of the supplementary material files, the Spectrum ID# uniquely identifies each fatty acid. Note that 6 spectra from each of the samples are included in the spectra database in a text files. Positive spectra are listed by #01488 - #01496 (01-03), and negative spectra by #01488 - #01496 (04-06). It was noted that in the positive ion spectra of Eicosatrienoic and Oleic acid, a peak matching M - H was seen. It is unclear how this ion forms.

SPECIMEN DESCRIPTION (ACCESSION #s 01488, 01489, 01490, 01491, 01492, 01493, 01494, 01495, 01496)

Host Material: Silicon (100) wafer

CAS Registry #: 7440-21-3

Host Material Characteristics: Homogeneous; solid; single crystal; semiconductor;

Chemical Name: Arachidic Acid (01488), Eicosatrienoic Acid (01489), Oleic Acid (01490), Linolenic Acid (01491), Palmitic Acid (01492), Palmitoleic Acid (01493), Sphingosine (01494), Stearic Acid (01495), Docosahexaenoic Acid (01496)

Source: Sigma-Aldrich Co, St. Louis, MO, USA

Host Composition: Si, SiO₂

Form: Arachidic Acid, Palmitic Acid, Palmitoleic Acid, Sphingosine, and Stearic Acid were crystalline powders

dissolved in ethanol; Eicosatrienoic Acid, Oleic Acid, Docosahexaenoic Acid and Linolenic Acid were liquid.

Lot Number: Arachidic Acid: BGBC3745, Eicosatrienoic Acid: SLBL3067V, Oleic Acid: SLBW3550, Linolenic Acid: SLBQ5256V, Palmitic Acid: SLBQ8866V, Palmitoleic Acid: SLBQ4106V, Sphingosine: MKBX9562V, Stearic Acid: BCBP3246V, Docosahexaenoic Acid: 0000036595

Structure: Arachidic Acid: C₂₀H₄₀O₂, Eicosatrienoic Acid: C₂₀H₃₄O₂, Oleic Acid: C₁₈H₃₄O₂, Linolenic Acid: C₁₈H₃₀O₂, Palmitic Acid: C₁₆H₃₂O₂, Palmitoleic Acid: C₁₆H₃₀O₂, Sphingosine: C₁₈H₃₇NO₂, Docosahexaenoic Acid: C₂₂H₃₂O₂, Stearic Acid: C₁₈H₃₆O₂,

History & Significance: Fatty acids and lipids are metabolic intermediate products in tissue homeostasis. Many cellular functions are dependent on the availability of lipids and fatty acids, particularly in cancer metabolism where specific fatty acids and lipids may be indicators of a cancerous state².

As Received Condition: Arachidic Acid, Palmitic Acid, Palmitoleic Acid, Sphingosine, and Stearic Acid were received in powder form; Eicosatrienoic Acid, Oleic Acid, Docosahexaenoic Acid and Linolenic Acid were received in liquid form

Analyzed Region: Areas of 500µm x 500µm with greatest coverage of specimen

Ex Situ Preparation/Mounting: For those in powder form, 20mg of each fatty acid was dissolved in 4mL of ethanol. 20 µl of these 5mg/mL fatty acid solutions were then deposited using a digital pipette onto the polished side of 1 cm x 1 cm cleaned silicon wafer. For those in liquid form, 20µL of each fatty acid was directly deposited using a digital pipette from its container onto the polished side of a 1 cm x 1 cm cleaned silicon wafer. All samples were then dried under vacuum at 226 mbar to facilitate crystallization.

In Situ Preparation: None

Charge Control: Low energy electrons

Temp. During Analysis: 291.15K

Pressure During Analysis: 2x10⁻⁷ Pa

Pre-Analysis Beam Exposure: None

INSTRUMENT CONFIGURATION

Manufacturer and Model: IONTOF, TOF.SIMS 5

Analyzer Type: time-of-flight

Experiment Type: mass spectrum

Sample Rotation: No

Rotation Rate: not rotated

Oxygen Flood Source: None

Oxygen Flood Pressure: N/A

Other Flood Source:

Other Flood Pressure: N/A

Unique Instrument Features Used: Time-of-Flight detector with grid less reflectron unit

Energy Acceptance Window: 14.3 eV

Postacceleration Voltage: 25 kV

Sample Bias: 0 eV

Specimen Normal-to-analyzer (Θ): 0°

Ion Sources

Ion Source 1 of 1

Purpose of this Ion Source: analysis beam

Ion Source Manufacturer: IONTOF (Münster, Germany)

Ion Source Model: 25 keV Bi cluster

Beam Mass Filter: yes

Describe Beam Mass Filter: Electrodynamic mass filter

Beam Species and Charge State: Bi₃⁺

Beam Gating Used: none

Additional Beam Comments: N/A

Beam Voltage: 25000 eV

Net Beam Voltage (impact voltage): 25000 eV

Ion Pulse Width: 17 ns

Ion Pulse Rate: 10 kHz

DC Beam Current: Not specified

Pulsed Beam Current: 0.0004 nA

Current Measurement Method: Faraday cup

Beam Diameter: 1 µm

Beam Raster Size: 500 µm x 500 µm

Beam Incident Angle: 45°

Source-to-Analyzer Angle: 45°

ACKNOWLEDGMENTS

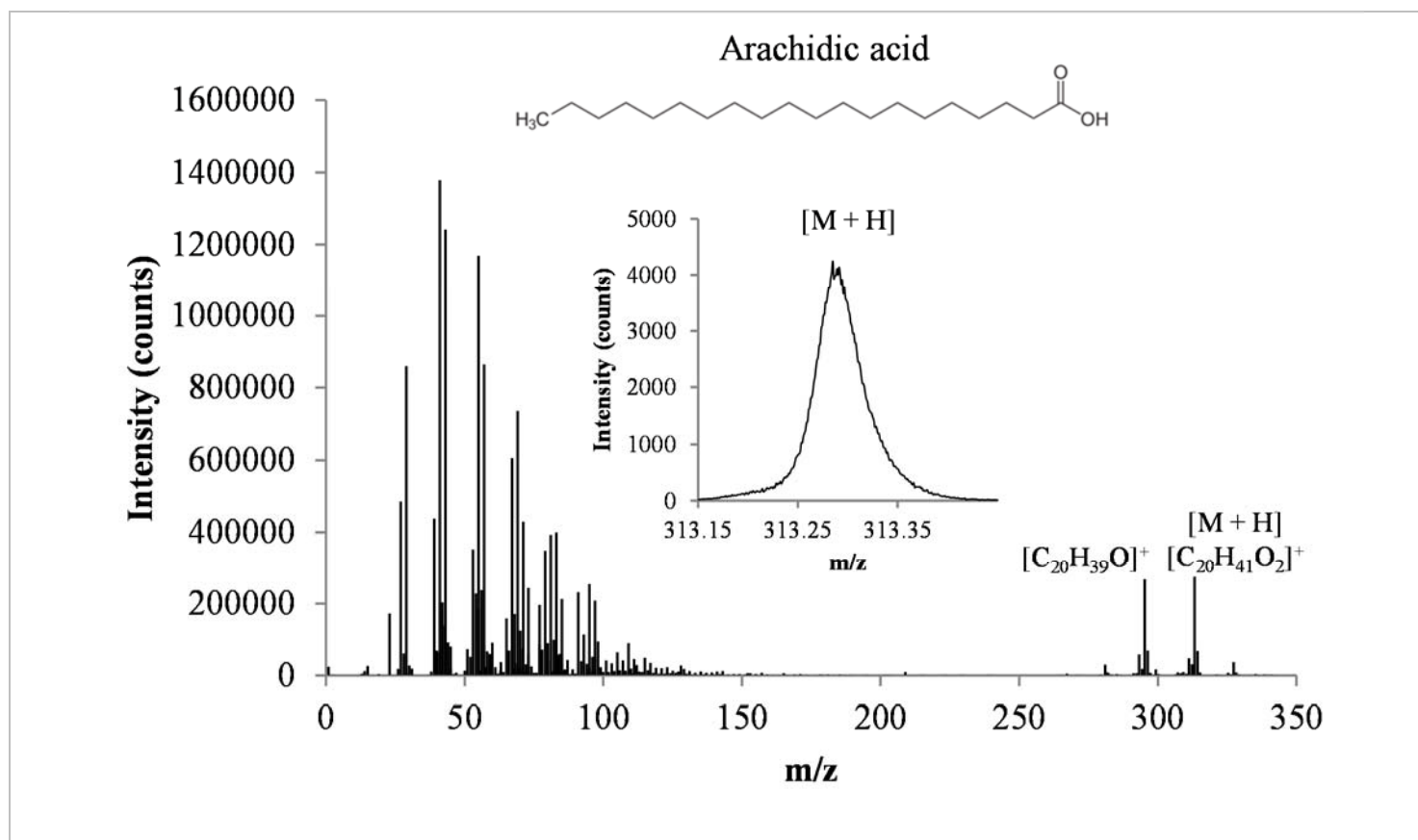
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REFERENCES

- (1) Passarelli, M. K.; Winograd, N. Lipid Imaging with Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS). *Biochim. Biophys. Acta - Mol. Cell Biol. Lipids* **2011**, *1811* (11), 976–990.
- (2) Bluestein, B. M.; Morrish, F.; Graham, D. J.; Huang, L.; Hockenbery, D.; Gamble, L. J. Analysis of the Myc-Induced Pancreatic β Cell Islet Tumor Microenvironment Using Imaging ToF-SIMS. *Biointerphases* **2018**, *13* (6), 06D402.

SPECTRAL FEATURES TABLE

Spectrum ID #	Mass (Da)	Species	Peak Assignment
01488 - 01	295.301	C ₂₀ H ₃₉ O ⁺	[M - H ₂ O + H]
	313.307	C ₂₀ H ₄₁ O ₂ ⁺	[M + H]

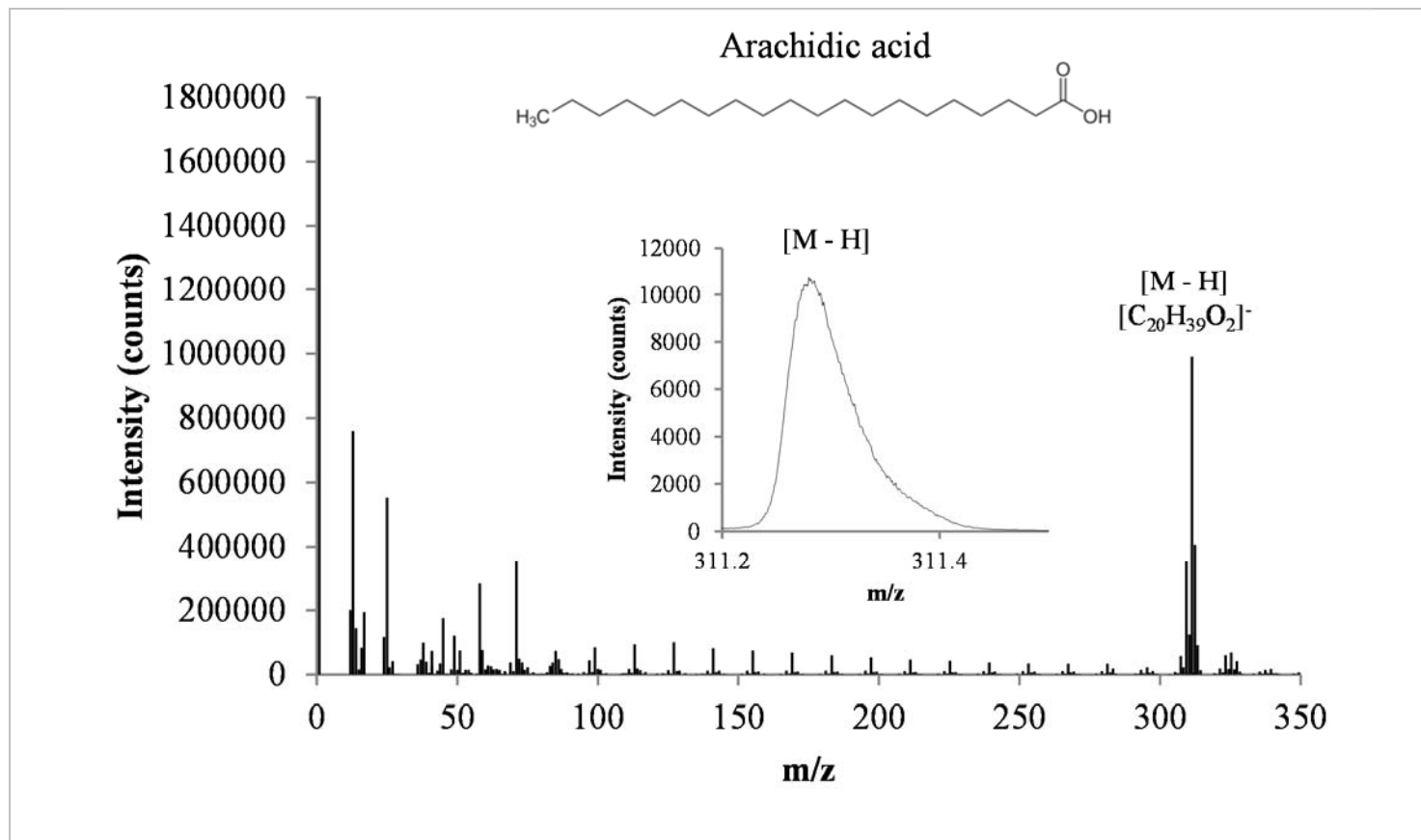


Accession # 01488-01, 01488-02, 01488-03

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	positive
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	CH ₃ ⁺ , C ₂ H ₃ ⁺ , C ₇ H ₉ ⁺
Analyzer Mass Resolution:	4106 m/Δm
Mass Resolution Determined at:	93 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ₃ ⁺
Primary Ion Dose:	6.1 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV

Pulsed Beam Current:	0.0004 nA
DC Beam Current:	Not specified
Beam Diameter:	1 μm
Beam Raster Size:	500 μm x 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 °
Source-to-Analyzer Angle:	45 °
Comment:	Enter comment.

Spectrum ID #	Mass (Da)	Species	Peak Assignment
01488 - 04	239.201	C ₁₅ H ₂₇ O ₂ ⁻	[M - H - C ₅ H ₁₀]
	253.218	C ₁₆ H ₂₉ O ₂ ⁻	[M - H - C ₄ H ₈]
	267.233	C ₁₇ H ₃₁ O ₂ ⁻	[M - H - C ₃ H ₆]
	281.248	C ₁₈ H ₃₃ O ₂ ⁻	[M - H - C ₂ H ₄]
	295.263	C ₁₉ H ₃₅ O ₂ ⁻	[M - H - CH ₂]
	311.295	C ₂₀ H ₃₉ O ₂ ⁻	[M - H]



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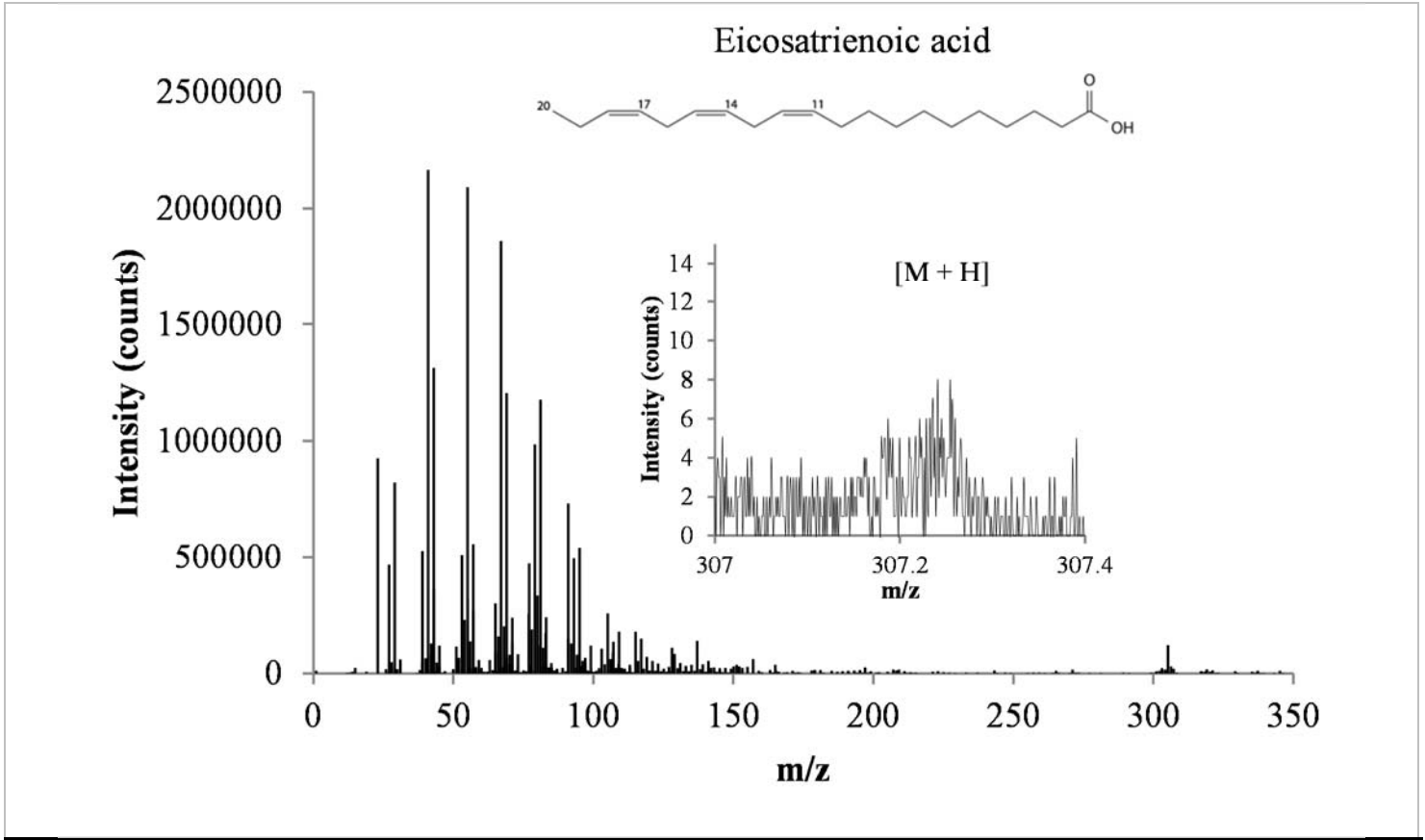
Accession #	01488-04, 01488-05, 01488-06
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■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	negative
Instrument:	ION-TOF, TOF-SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	CH ⁻ , C ₂ H ⁻ , C ₄ H ⁻
Analyzer Mass Resolution:	6568 m/Δm
Mass Resolution Determined at:	61 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ₃ ⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns

Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV
Pulsed Beam Current:	0.0004 nA
DC Beam Current:	nA
Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Repeat CH ₂ loss in spectra from deprotonated parent ion

Eicosatrienoic Acid

Spectrum ID #	Mass (Da)	Species	Peak Assignment
01489 - 01	305.248	C ₂₀ H ₃₃ O ₂ ⁺



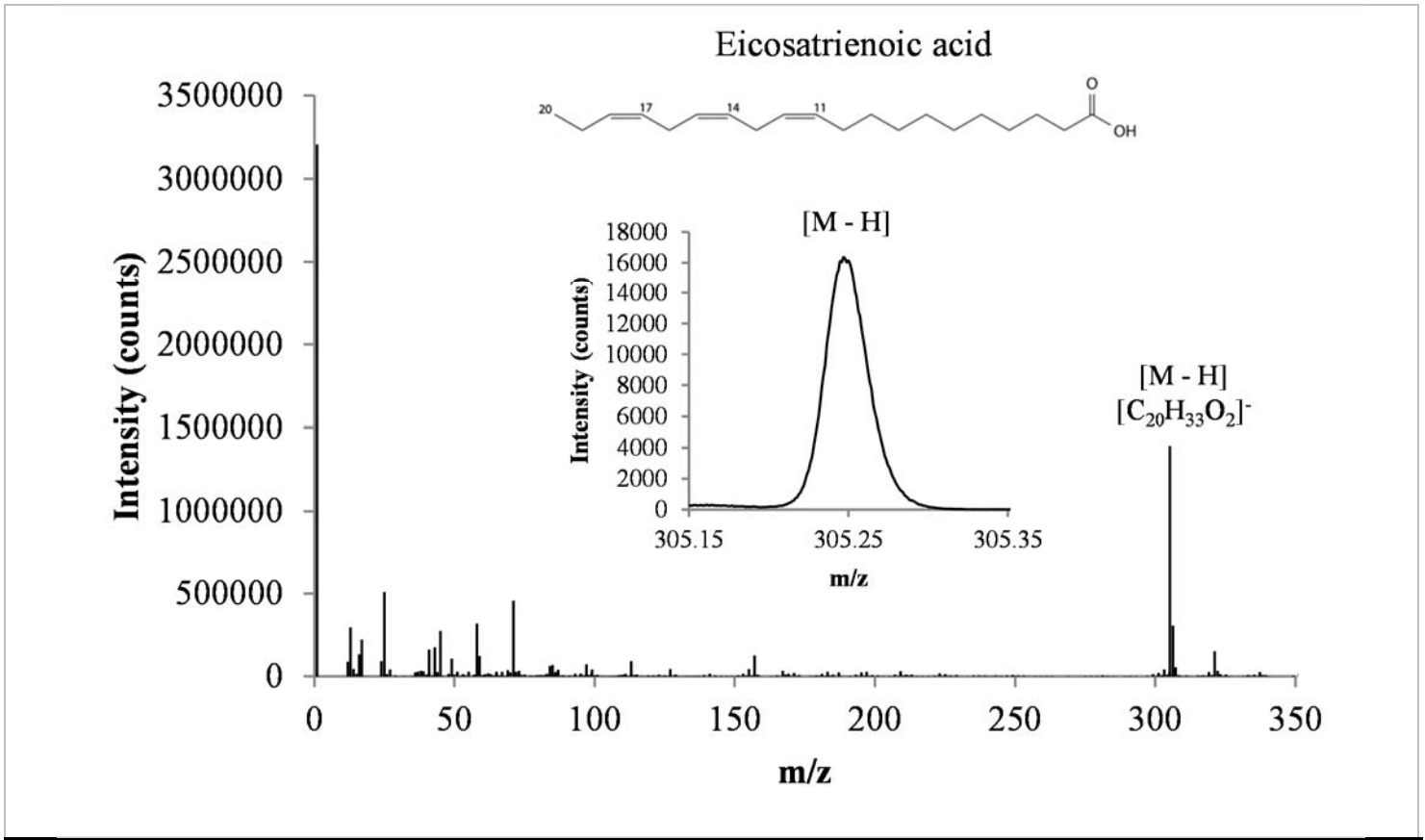
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■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	positive
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	CH ₃ ⁺ , C ₂ H ₃ ⁺ , C ₇ H ₉ ⁺
Analyzer Mass Resolution:	3981 m/Δm
Mass Resolution Determined at:	93.067 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	49 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ³⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV
Pulsed Beam Current:	0.0004 nA

DC Beam Current:	nA
Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Possible formation of M – H in positive polarity

Eicosatrienoic Acid

Spectrum ID #	Mass (Da)	Species	Peak Assignment
01489 - 04	305.248	C ₂₀ H ₃₃ O ₂ ⁻	[M - H]



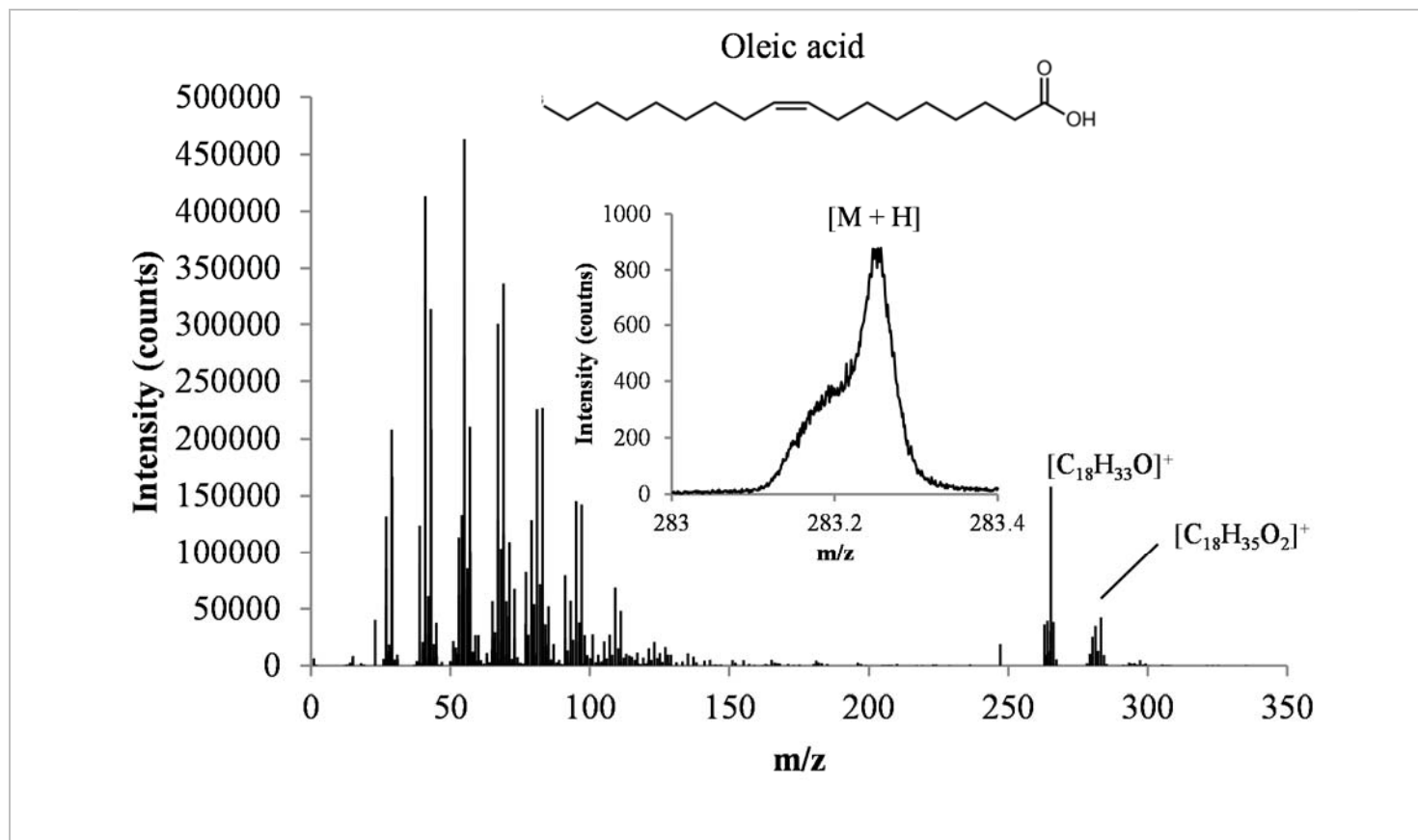
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01489-04, 01489-05, 01489-06

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	negative
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	CH ⁻ , C ₂ H ⁻ , C ₄ H ⁻
Analyzer Mass Resolution:	6254 m/Δm
Mass Resolution Determined at:	61 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	49 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ₃ ⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV
Pulsed Beam Current:	0.0004 nA
DC Beam Current:	Not specified

Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	No loss of CH ₂ repeat from M - H

Oleic Acid			
Spectrum ID #	Mass (Da)	Species	Peak Assignment
01490 - 01	265.249	$C_{18}H_{33}O^+$	$[M - H_2O + H]$
	283.264	$C_{18}H_{35}O_2^+$	$[M + H]$



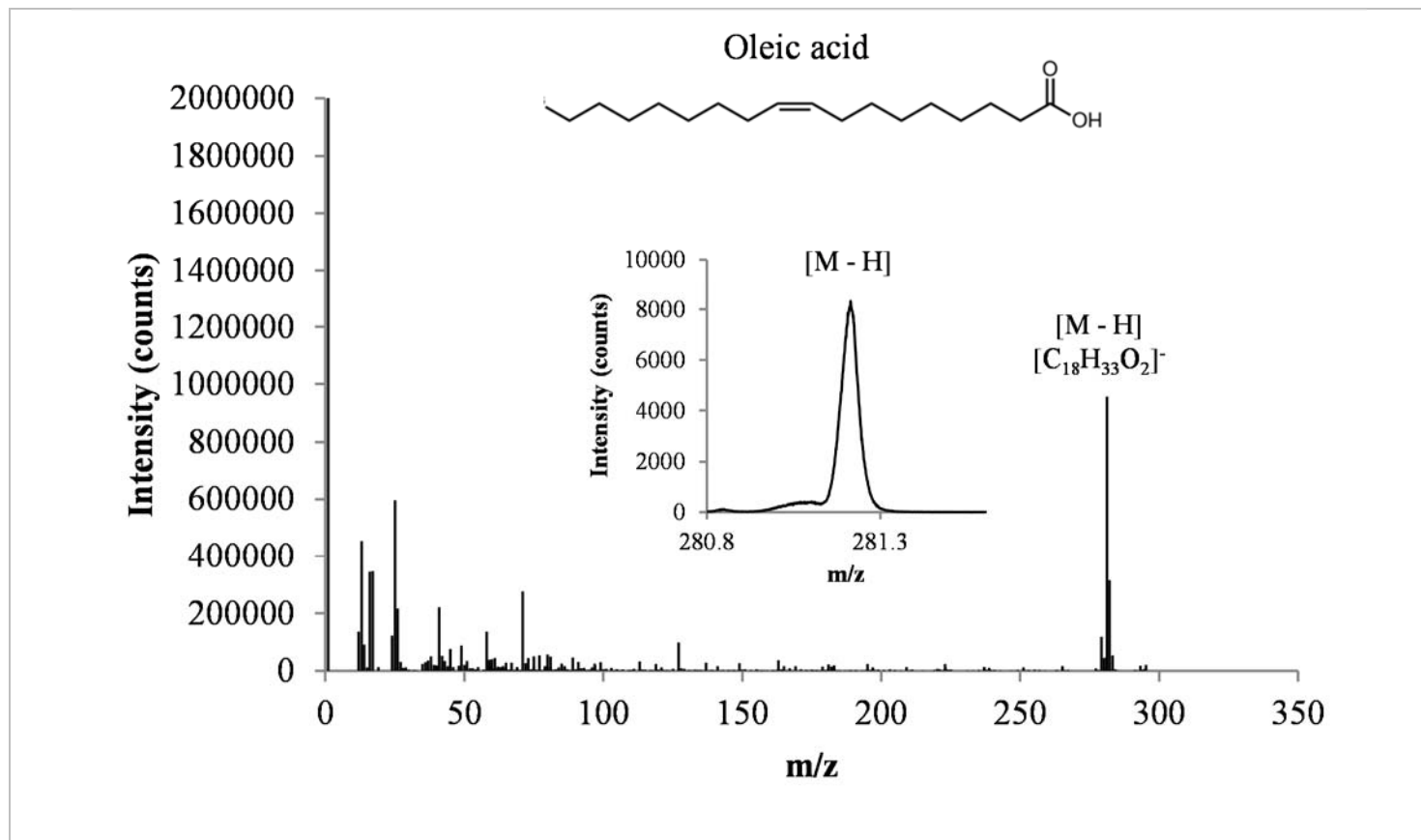
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■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	positive
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	CH_3^+ , $C_2H_3^+$, $C_7H_9^+$
Analyzer Mass Resolution:	4028 m/Δm
Mass Resolution Determined at:	93 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	49 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi_3^+
Primary Ion Dose:	6.14×10^{10} ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV

Pulsed Beam Current:	0.0004 nA
DC Beam Current:	nA
Beam Diameter:	Not specified
Beam Raster Size:	500 μ m \times 500 μ m
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 °
Source-to-Analyzer Angle:	45 °
Comment:	Enter comment.

Oleic Acid			
Spectrum ID #	Mass (Da)	Species	Peak Assignment
01490 - 04	281.246	$C_{18}H_{33}O_2^-$	[M - H]



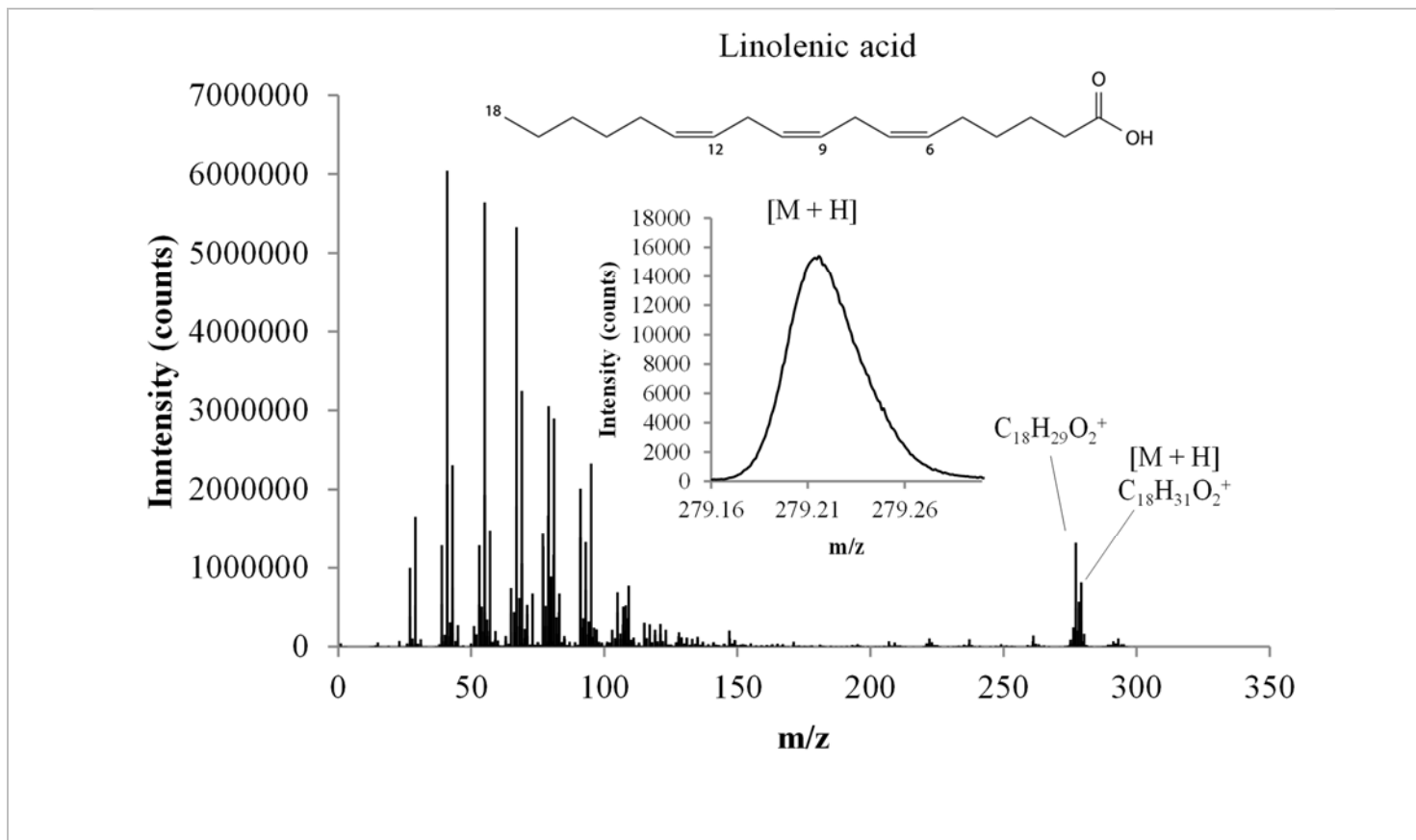
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01490-04, 01490-05, 01490-06

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	negative
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	CH ⁻ , OH ⁻ , C ₂ H ⁻ , C ₄ H ⁻
Analyzer Mass Resolution:	6982 m/Δm
Mass Resolution Determined at:	61 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	49 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ₃ ⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV
Pulsed Beam Current:	0.0004 nA
DC Beam Current:	Not specified

Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Enter comment.

Linolenic Acid			
Spectrum ID #	Mass (Da)	Species	Peak Assignment
01491 - 01	277.214	C ₁₈ H ₂₉ O ₂ ⁺
	279.231	C ₁₈ H ₃₁ O ₂ ⁺	[M + H]



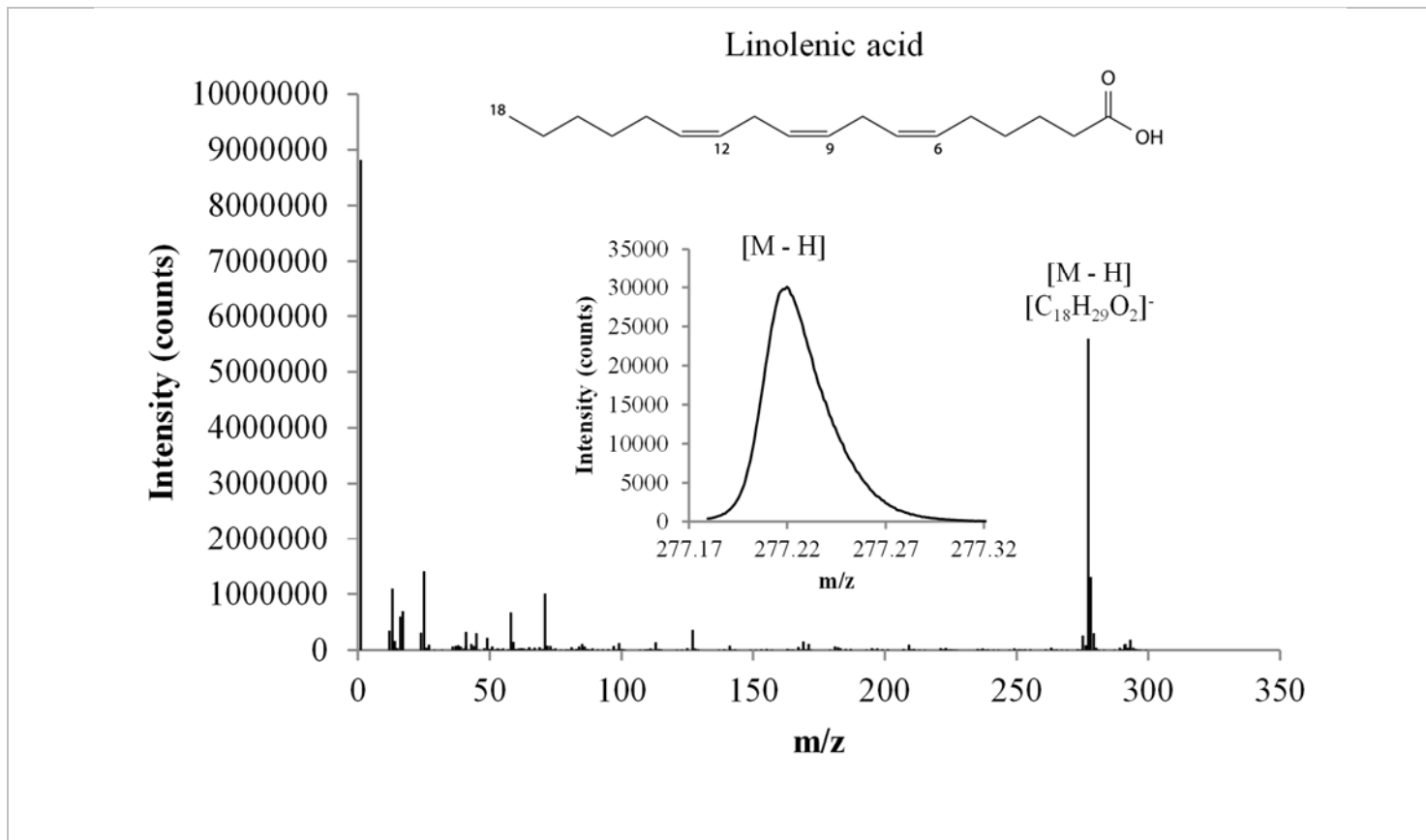
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01491-01, 01491-02, 01491-03

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	positive
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	CH ₃ ⁺ , C ₂ H ₃ ⁺ , C ₈ H ₉ ⁺
Analyzer Mass Resolution:	4823 m/Δm
Mass Resolution Determined at:	93 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ₃ ⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV
Pulsed Beam Current:	0.0004 nA

DC Beam Current:	Not specified
Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Enter comment.

Linolenic Acid			
Spectrum ID #	Mass (Da)	Species	Peak Assignment
01491 - 04	235.170	C ₁₅ H ₂₃ O ₂ ⁻
	249.183	C ₁₆ H ₂₅ O ₂ ⁻
	263.201	C ₁₇ H ₂₇ O ₂ ⁻
	277.216	C ₁₈ H ₂₉ O ₂ ⁻	[M - H]



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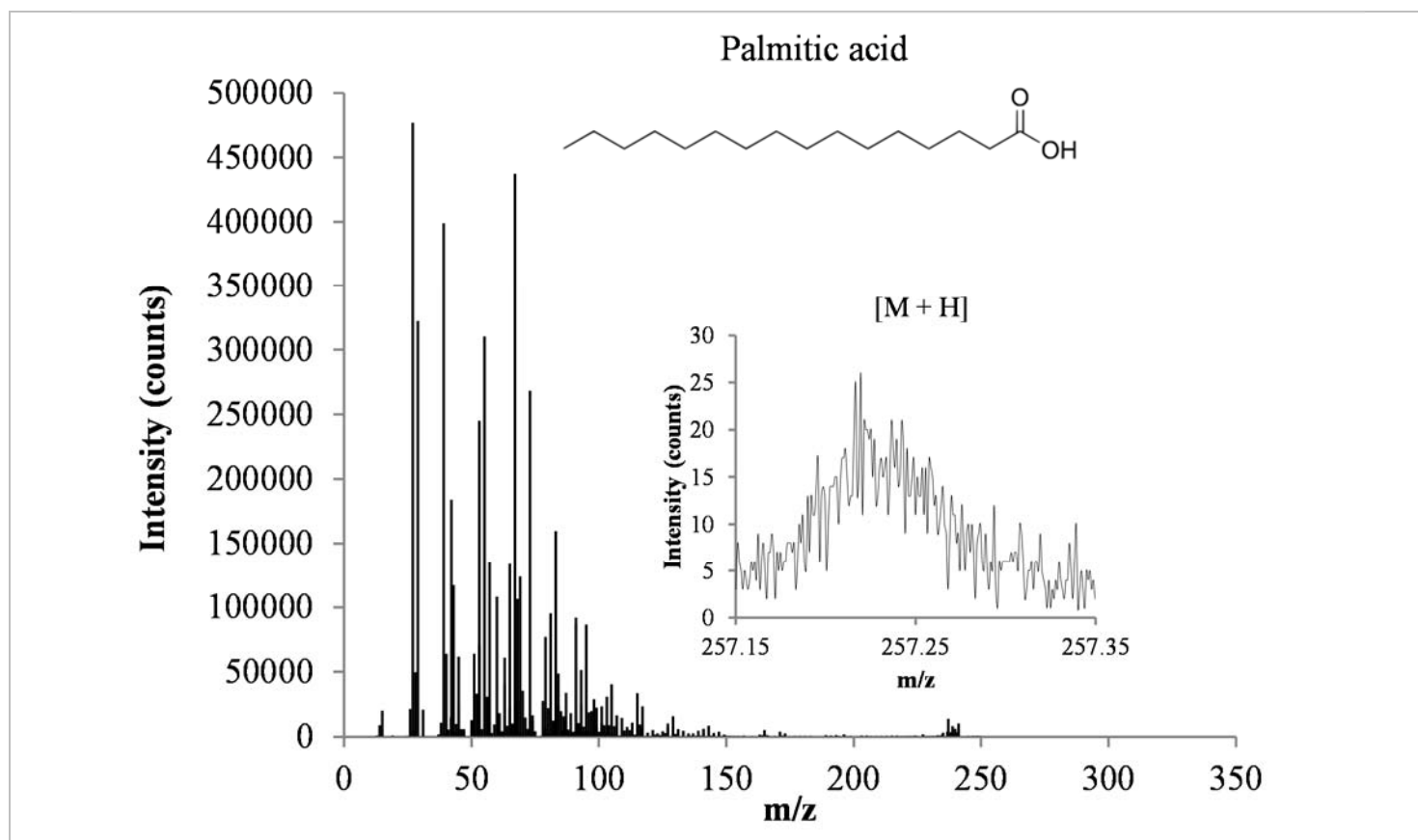
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01491-04, 01491-05, 01491-06

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	negative
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	CH ⁺ , OH ⁺ , C ₂ H ⁺ , C ₄ H ⁺ , C ₅ H ⁺
Analyzer Mass Resolution:	6192 m/Δm
Mass Resolution Determined at:	61 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ₃ ⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV

Pulsed Beam Current:	0.0004 nA
DC Beam Current:	nA
Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Enter comment.

Palmitic Acid			
Spectrum ID #	Mass (Da)	Species	Peak Assignment
01492 - 01	237.222	C ₁₆ H ₂₉ O ⁺	[M + H - H ₂ O]
	253.217	C ₁₆ H ₂₉ O ₂ ⁺
	257.248	C ₁₆ H ₃₃ O ₂ ⁺



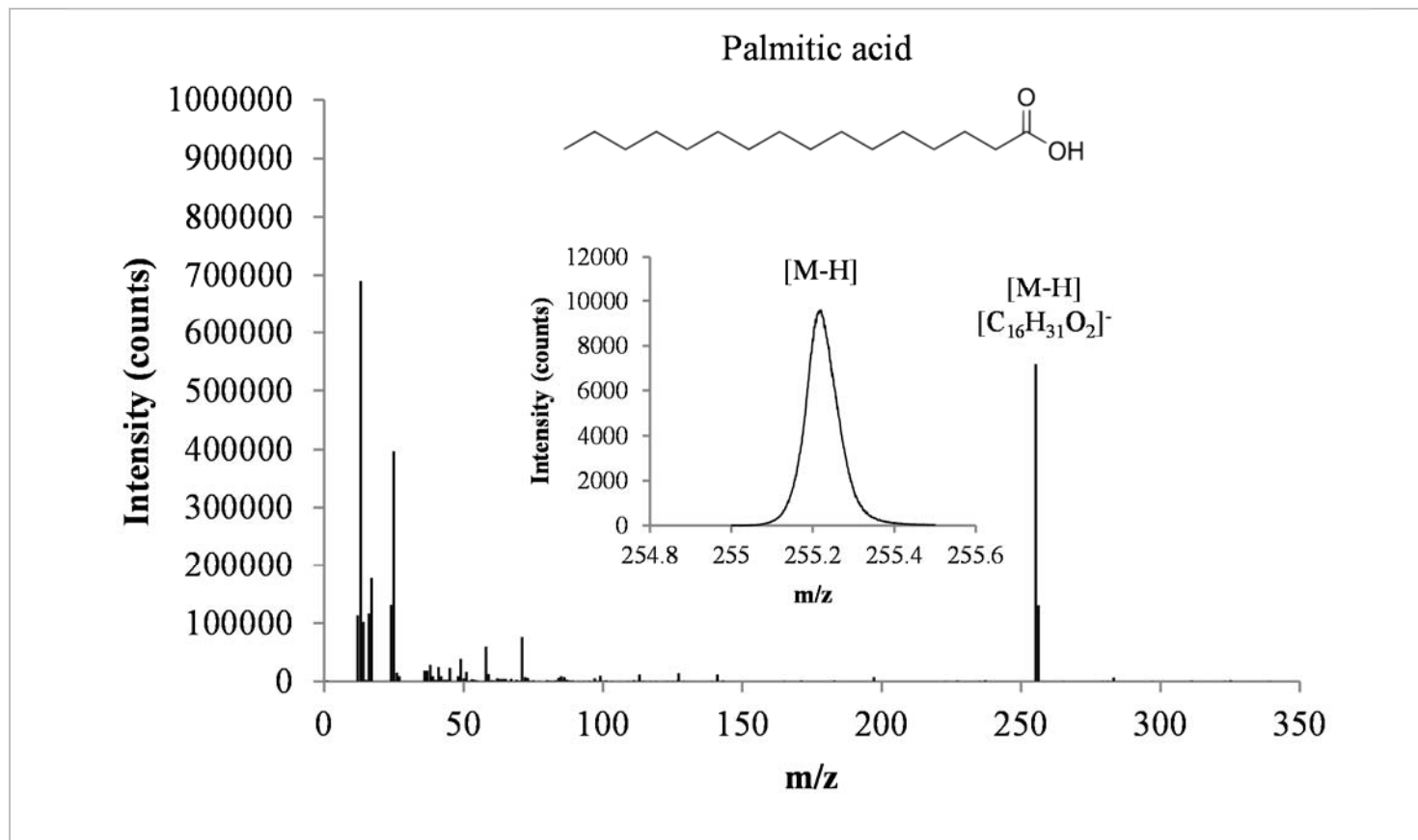
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01492-01, 01491-02, 01491-03

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	positive
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	CH ₃ ⁺ , C ₂ H ₃ ⁺ , C ₇ H ₉ ⁺
Analyzer Mass Resolution:	5621 m/Δm
Mass Resolution Determined at:	93 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ₃ ⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV

Pulsed Beam Current:	0.0004 nA
DC Beam Current:	Not specified
Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Enter comment.

Palmitic Acid			
Spectrum ID #	Mass (Da)	Species	Peak Assignment
01492 - 04	253.218	C ₁₆ H ₂₉ O ₂ ⁻
	255.234	C ₁₆ H ₃₁ O ₂ ⁻	M - H



Accession #

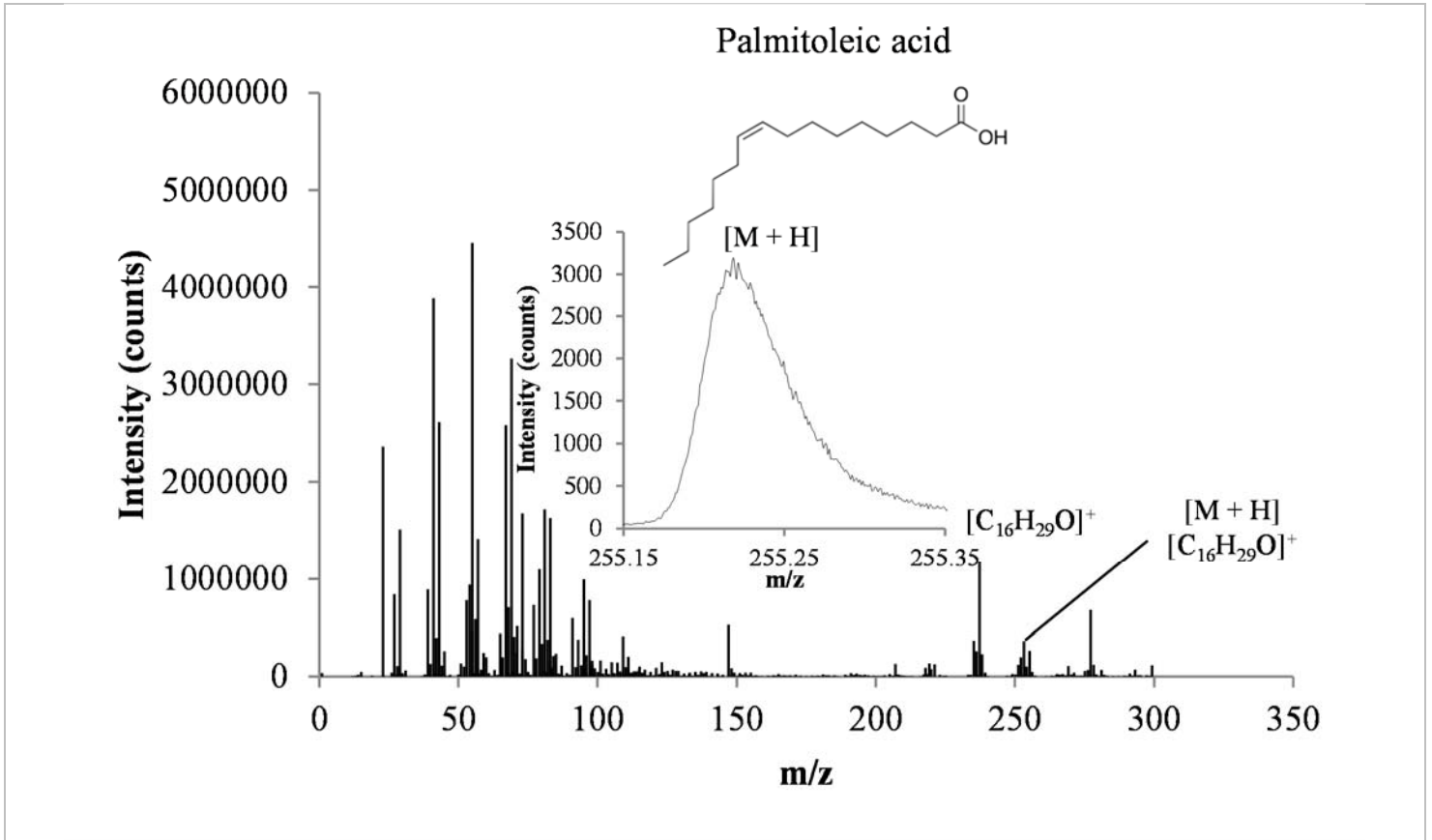
01492-04, 01491-05, 01491-06

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	negative
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	OH ⁻ , C ₂ H ⁻ , C ₄ H ⁻
Analyzer Mass Resolution:	5514 m/Δm
Mass Resolution Determined at:	61 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ₃ ⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV
Pulsed Beam Current:	0.0004 nA

DC Beam Current:	Not specified
Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Enter comment.

Palmitoleic Acid

Spectrum ID #	Mass (Da)	Species	Peak Assignment
01493 - 01	237.220	C ₁₆ H ₂₉ O ⁺	[M + H - H ₂ O]
	251.198	C ₁₆ H ₂₇ O ₂ ⁺
	253.215	C ₁₆ H ₂₉ O ₂ ⁺
	254.225	C ₁₆ H ₃₀ O ₂ ⁺	M
	255.245	C ₁₆ H ₃₁ O ₂ ⁺	M + H
	277.206	C ₁₆ H ₃₀ O ₂ ⁺	M + Na



Accession #

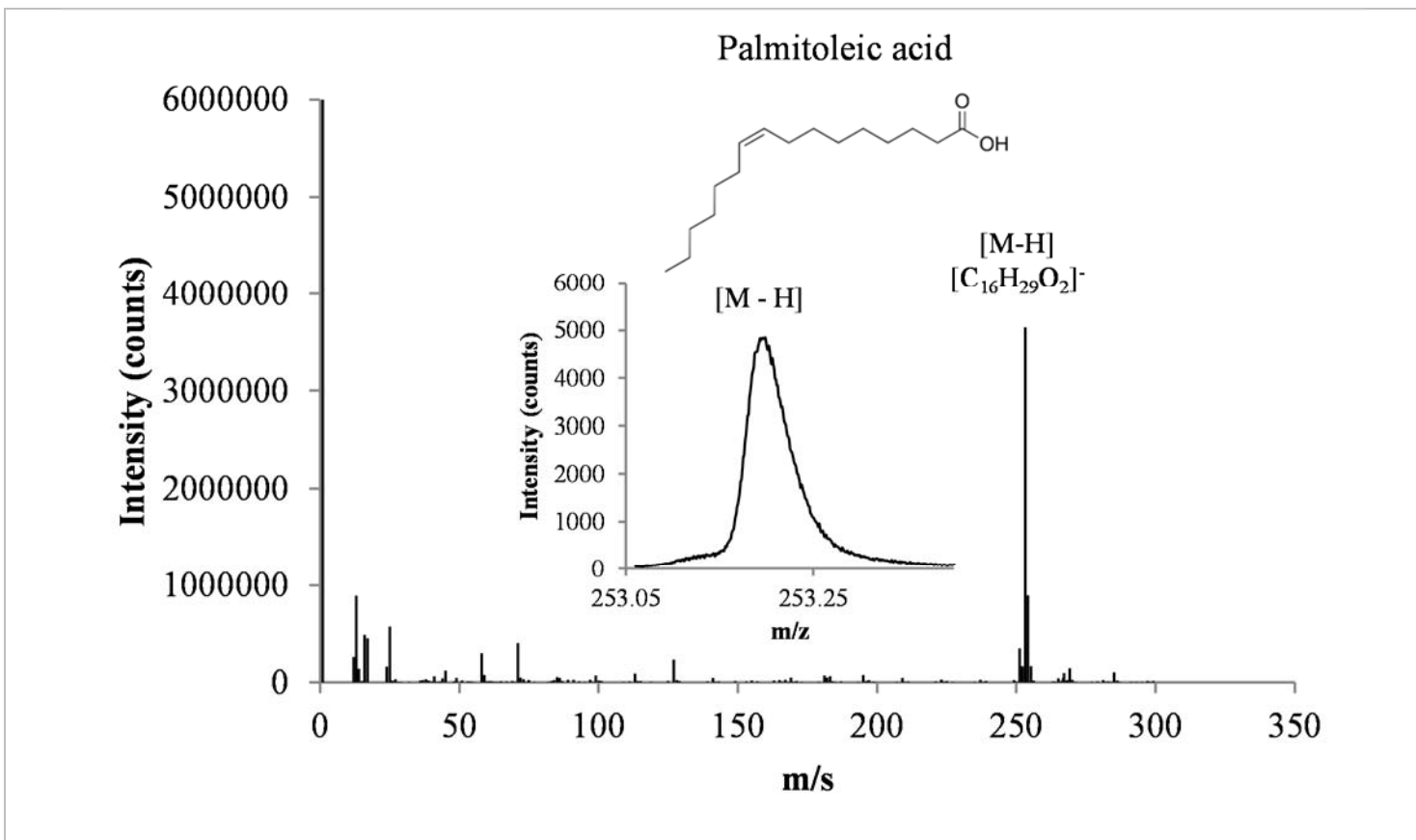
01493-01, 01493-02, 01493-03

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	positive
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	CH ₃ ⁺ , C ₂ H ₃ ⁺ , C ₇ H ₉ ⁺
Analyzer Mass Resolution:	4023 m/Δm
Mass Resolution Determined at:	93 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ₃ ⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns

Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV
Pulsed Beam Current:	0.0004 nA
DC Beam Current:	Not specified
Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Enter comment.

Palmitoleic Acid

Spectrum ID #	Mass (Da)	Species	Peak Assignment
01493 - 04	237.185	C ₁₅ H ₂₅ O ₂ ⁻
	251.198	C ₁₆ H ₂₇ O ₂ ⁻
	253.217	C ₁₆ H ₂₉ O ₂ ⁻	M - H



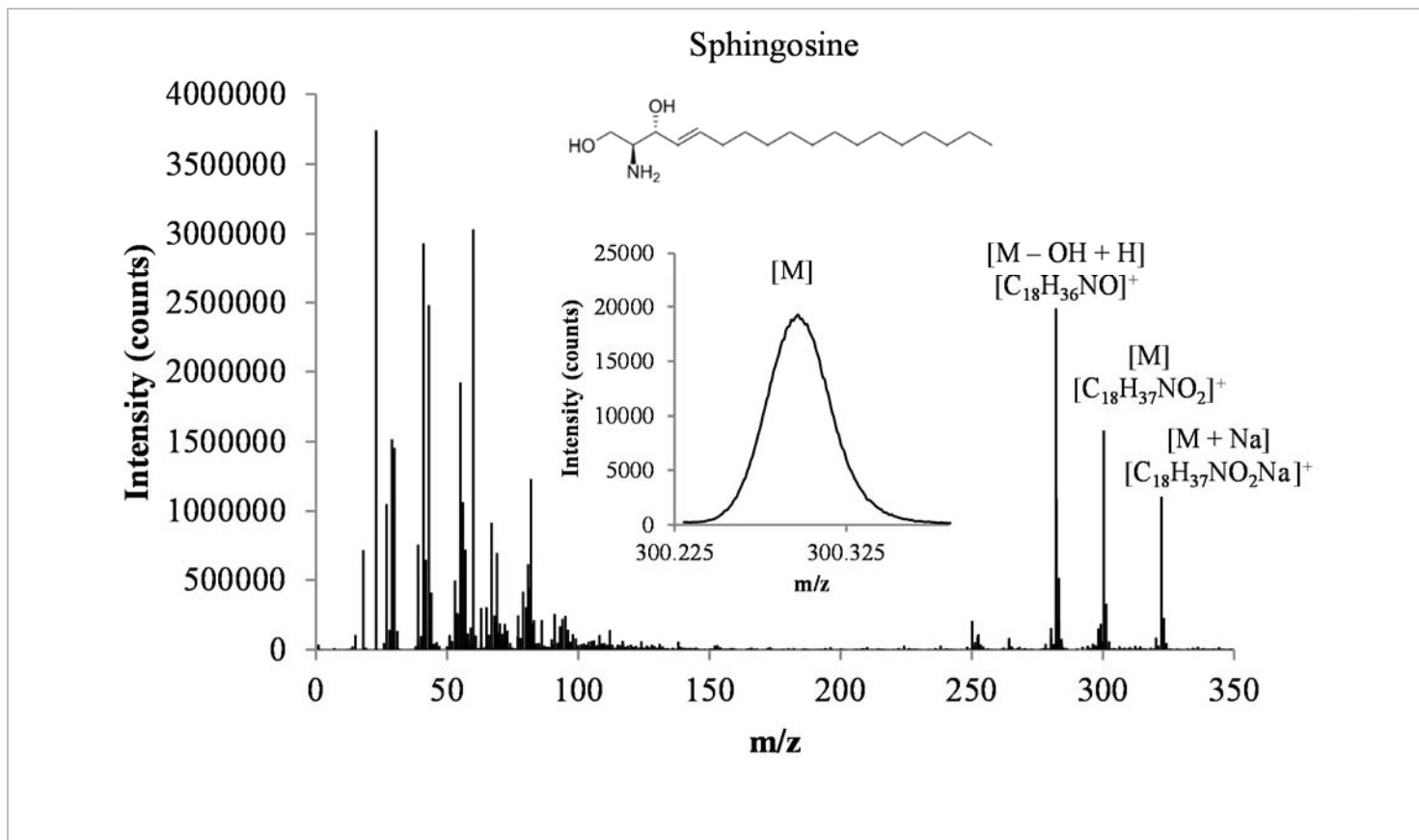
Accession #

01493-04, 01493-05, 01493-06

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	negative
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	OH ⁻ , C ₂ H ⁻ , C ₄ H ⁻
Analyzer Mass Resolution:	6041 m/Δm
Mass Resolution Determined at:	61 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ₃ ⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV

Pulsed Beam Current:	0.0004 nA
DC Beam Current:	Not specified
Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Enter comment.

Sphingosine			
Spectrum ID #	Mass (Da)	Species	Peak Assignment
01494 - 01	196.143	C ₁₂ H ₂₀ O ₂ ⁺
	210.164	C ₁₃ H ₂₂ O ₂ ⁺
	224.181	C ₁₄ H ₂₄ O ₂ ⁺
	281.271	C ₁₈ H ₃₆ NO ⁺	[M - OH + H]
	299.282	C ₁₈ H ₃₇ NO ₂ ⁺	[M]
	322.272	C ₁₈ H ₃₇ NO ₂ Na ⁺	[M] + Na

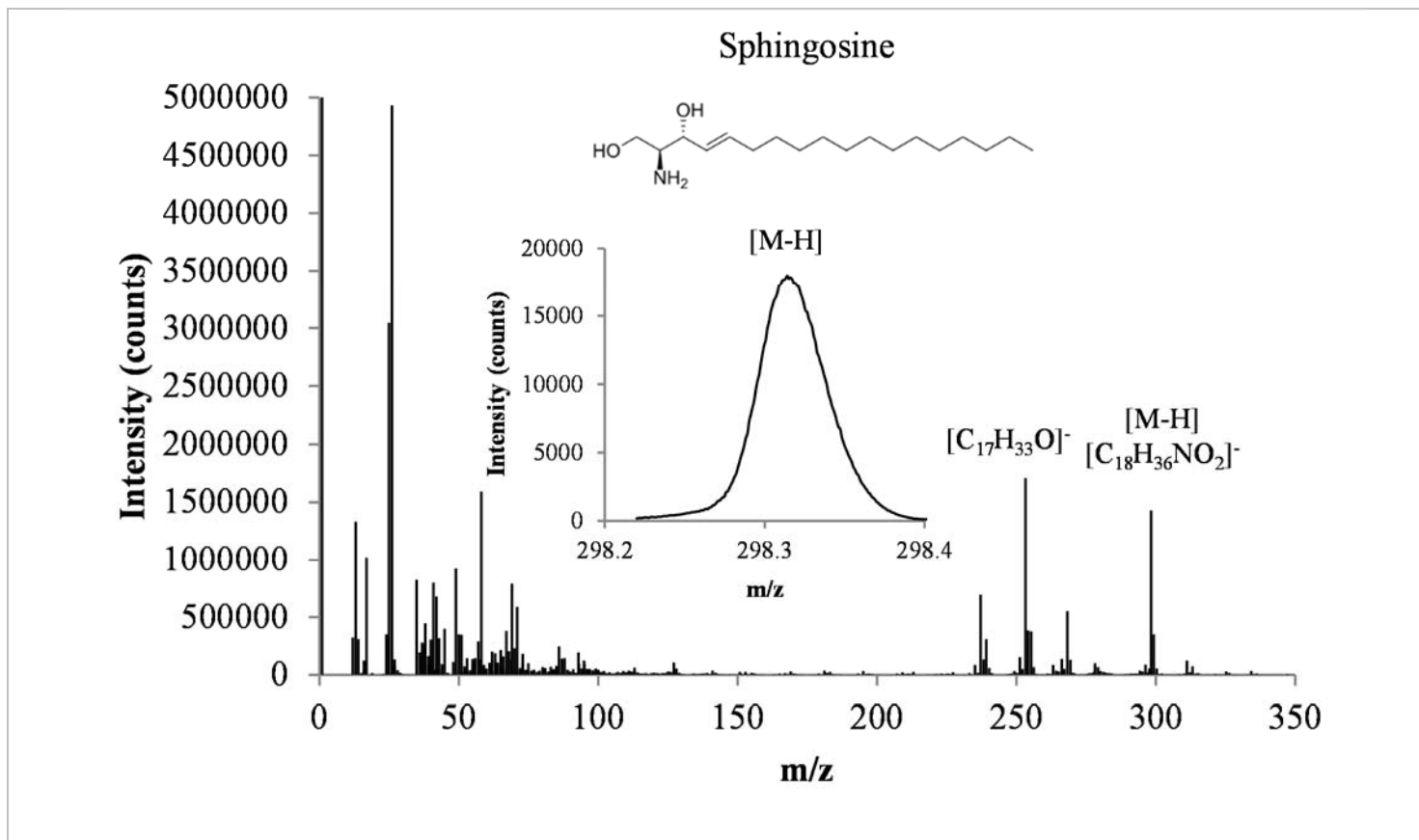


Accession # **01494-01, 01494-02, 01494-03**

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	positive
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	CH ₃ ⁺ , C ₂ H ₃ ⁺ , C ₇ H ₉ ⁺
Analyzer Mass Resolution:	6128 m/Δm
Mass Resolution Determined at:	93 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ³⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns

Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV
Pulsed Beam Current:	0.0004 nA
DC Beam Current:	Not specified
Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Na ⁺ peak intensity has scaled by half in spectra

Sphingosine			
Spectrum ID #	Mass (Da)	Species	Peak Assignment
01494 - 04	253.253	$C_{17}H_{33}O^-$
	298.275	$C_{18}H_{36}NO_2^-$	M - H



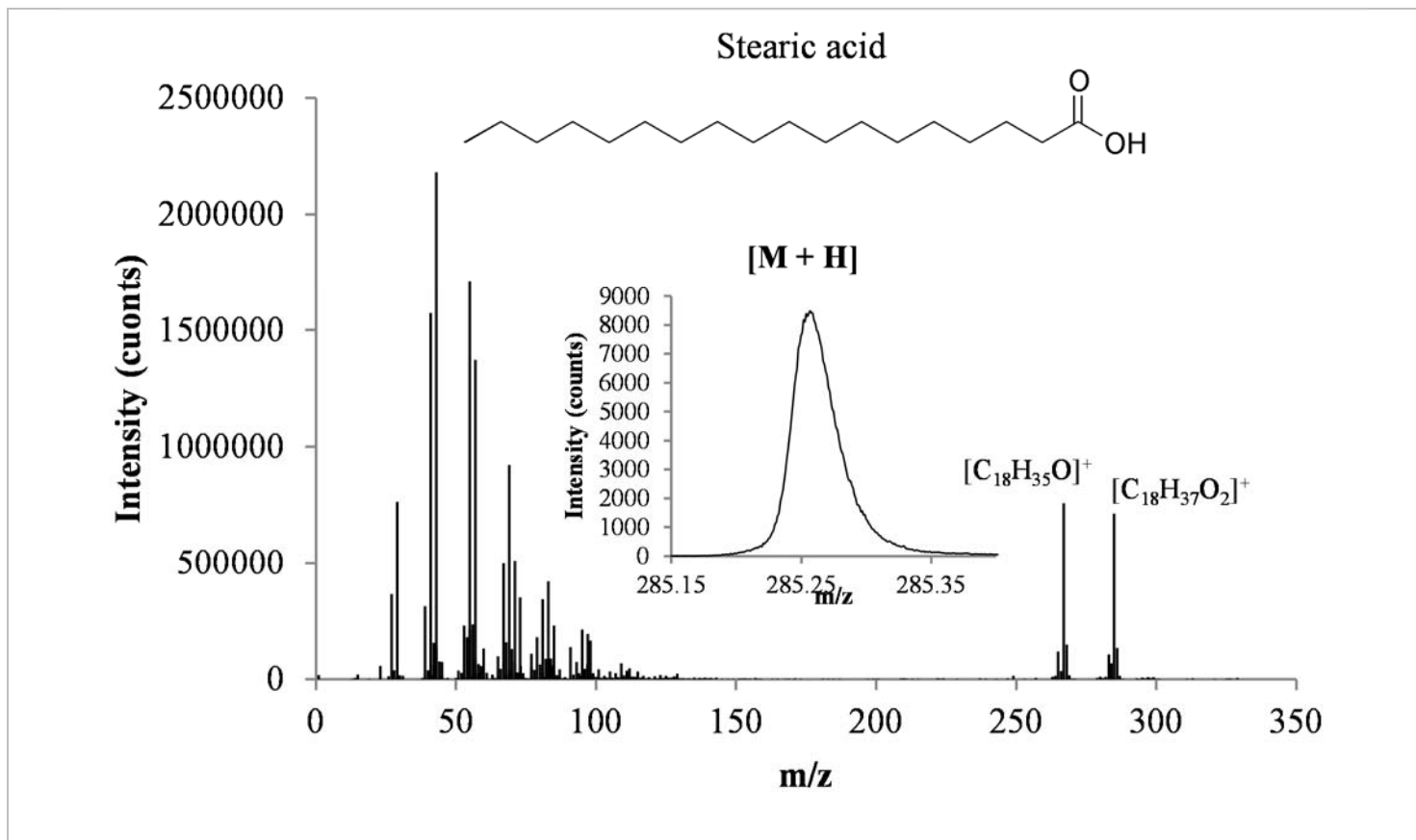
21 April 2025 21:30:41

Accession # 01494-04, 01494-05, 01494-06

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	negative
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	OH^- , C_4H^- , C_5H^-
Analyzer Mass Resolution:	5805 m/Δm
Mass Resolution Determined at:	61 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi_3^+
Primary Ion Dose:	6.14×10^{10} ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV
Pulsed Beam Current:	0.0004 nA

DC Beam Current:	Not specified
Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Enter comment.

Stearic Acid			
Spectrum ID #	Mass (Da)	Species	Peak Assignment
01495 - 01	267.273	C ₁₈ H ₃₅ O ⁺	[M - H ₂ O + H]
	285.278	C ₁₈ H ₃₇ O ₂ ⁺	[M + H]



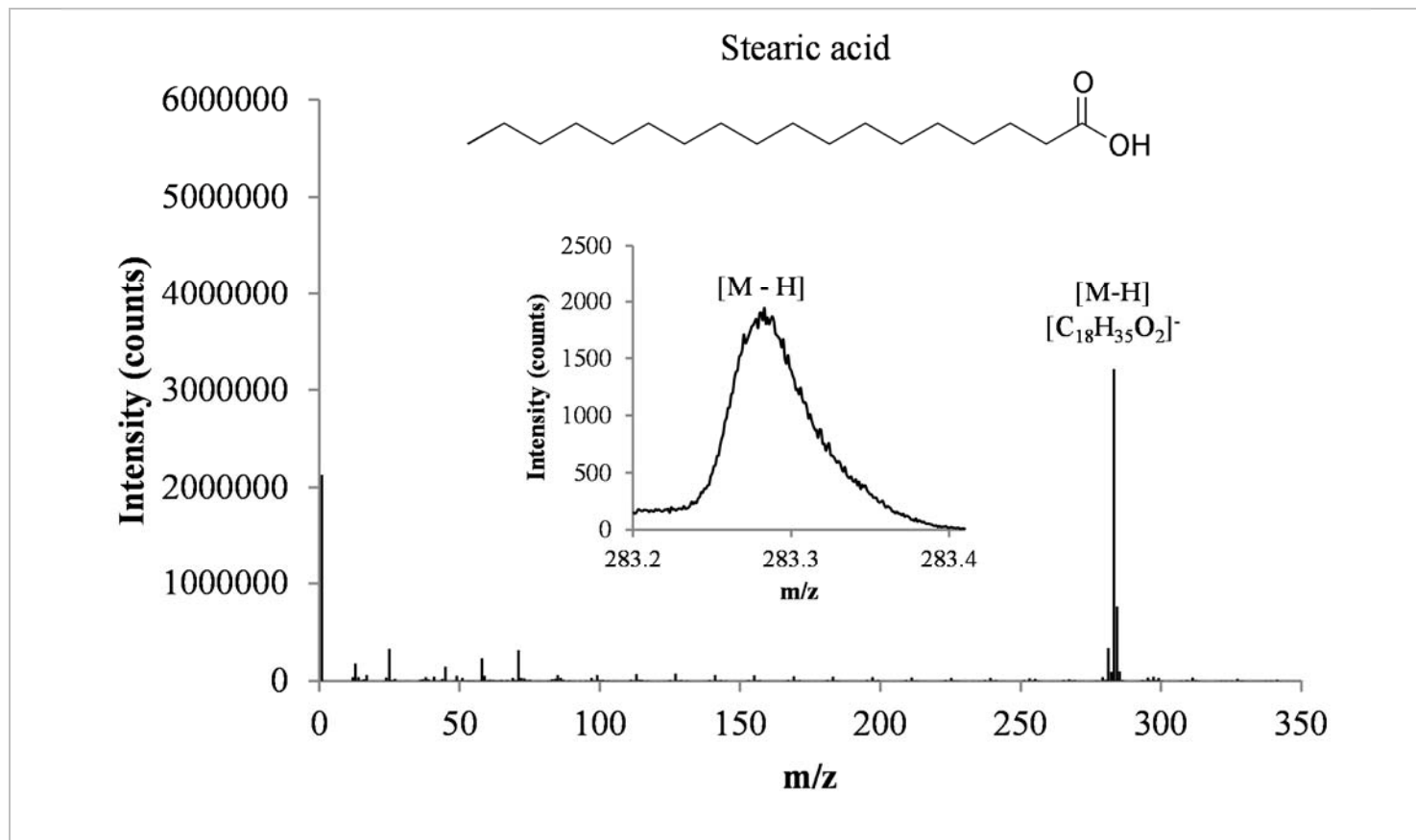
Accession #

01495-01, 01495-02, 01495-03

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	positive
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	C ₄ H ₅ ⁺ , C ₅ H ₆ ⁺ , C ₇ H ₉ ⁺
Analyzer Mass Resolution:	3824 m/Δm
Mass Resolution Determined at:	93 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ₃ ⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV
Pulsed Beam Current:	0.0004 nA

DC Beam Current:	nA
Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Enter comment.

Stearic Acid			
Spectrum ID #	Mass (Da)	Species	Peak Assignment
01495 - 04	283.264	$C_{18}H_{35}O_2^-$	[M - H]



Accession #

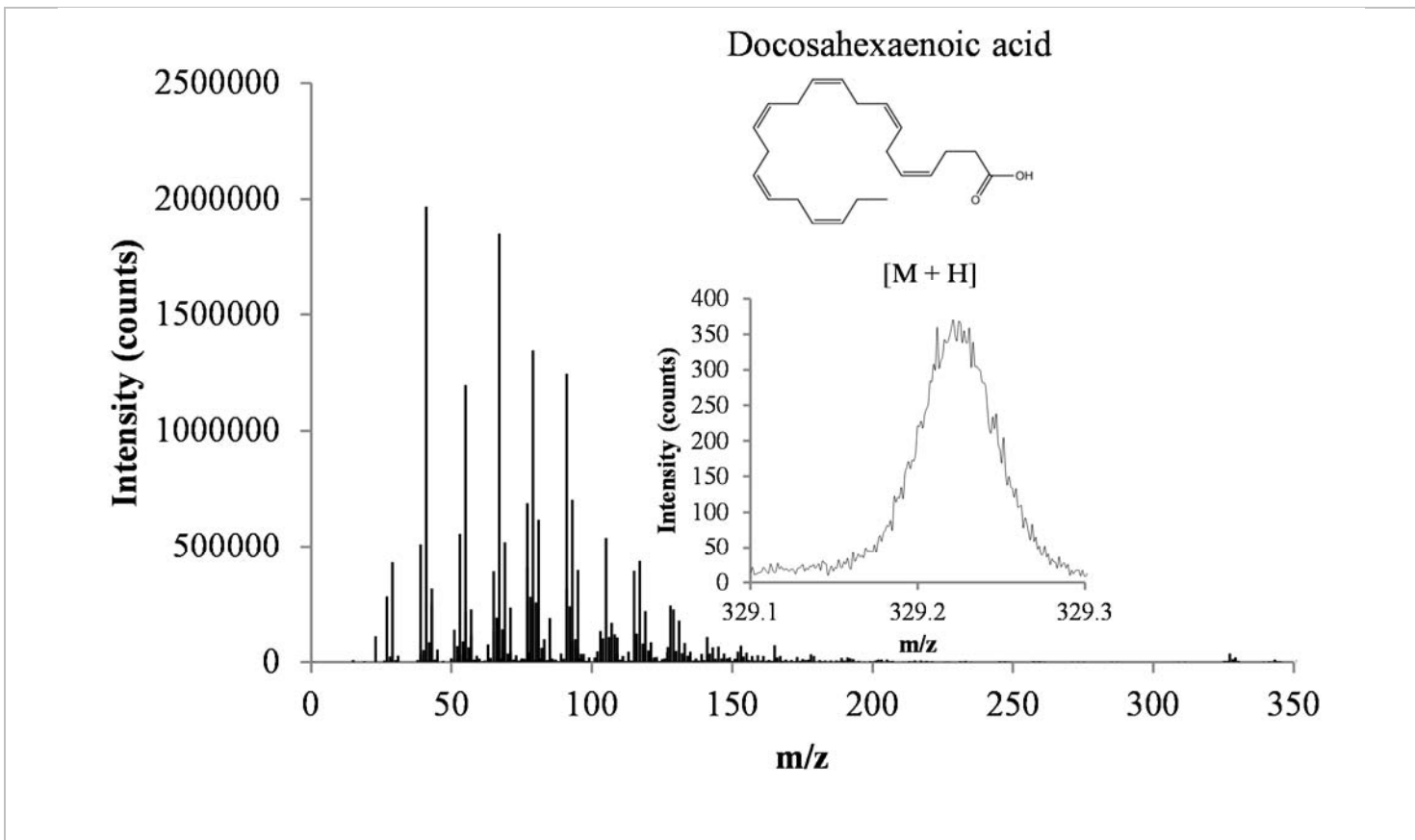
01495-04, 01495-05, 01495-06

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	negative
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	CH^+ , OH^- , C_5H^+
Analyzer Mass Resolution:	6028 m/Δm
Mass Resolution Determined at:	61 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi_3^+
Primary Ion Dose:	6.14×10^{10} ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV
Pulsed Beam Current:	0.0004 nA

DC Beam Current:	Not specified
Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Enter comment.

Docosahexaenoic acid

Spectrum ID #	Mass (Da)	Species	Peak Assignment
01496 - 01	327.232 329.247	C ₂₂ H ₃₁ O ₂ ⁺ C ₂₂ H ₃₃ O ₂ ⁺ [M + H]



Accession #

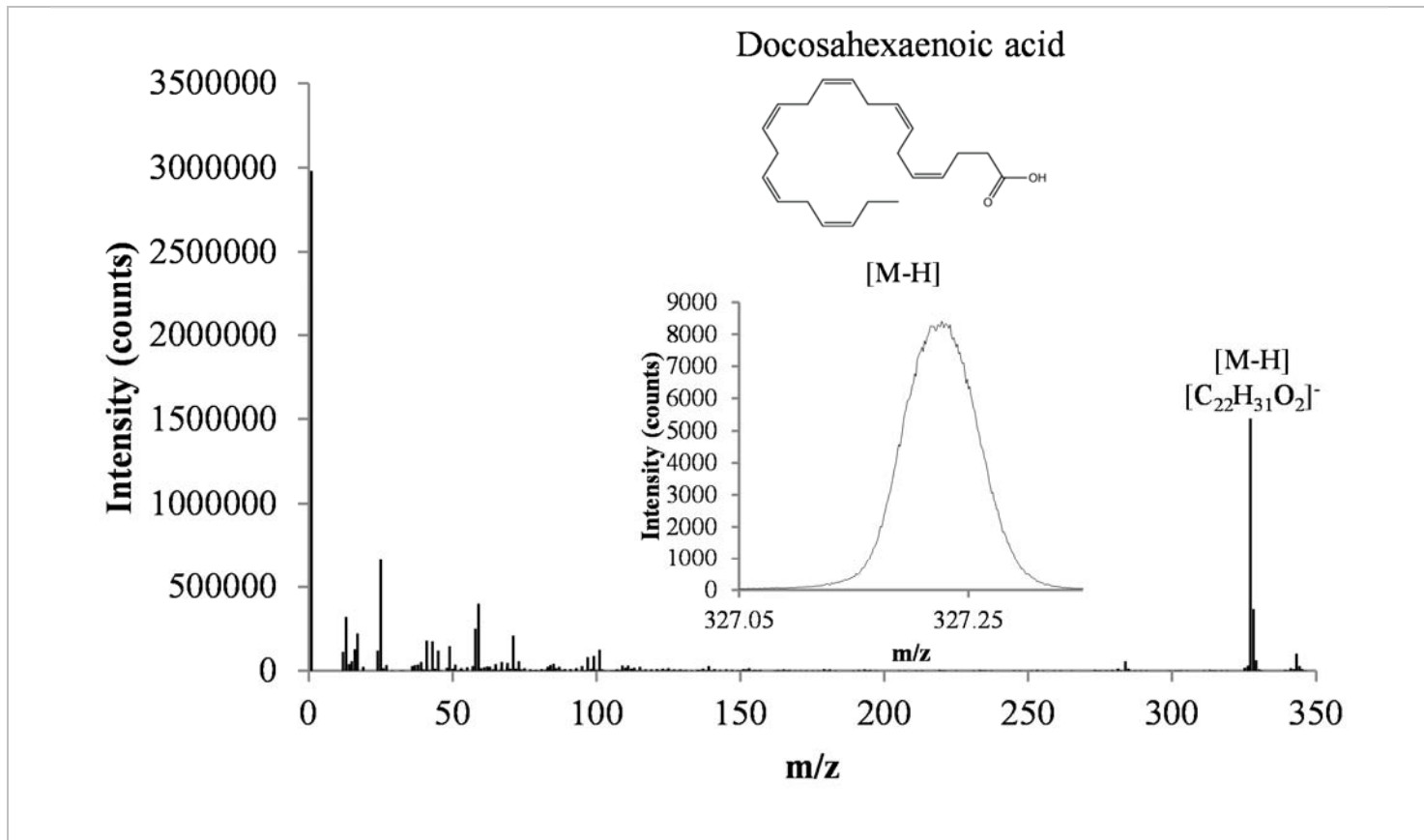
01495-01, 01495-02, 01495-03

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	positive
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	C ₄ H ₅ ⁺ , C ₅ H ₆ ⁺ , C ₇ H ₉ ⁺
Analyzer Mass Resolution:	4358 m/Δm
Mass Resolution Determined at:	93 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ₃ ⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV
Pulsed Beam Current:	0.0004 nA

DC Beam Current:	nA
Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Enter comment.

Docosahexaenoic acid

Spectrum ID #	Mass (Da)	Species	Peak Assignment
01496 - 04	327.231	C ₂₂ H ₃₁ O ₂ ⁻	M - H



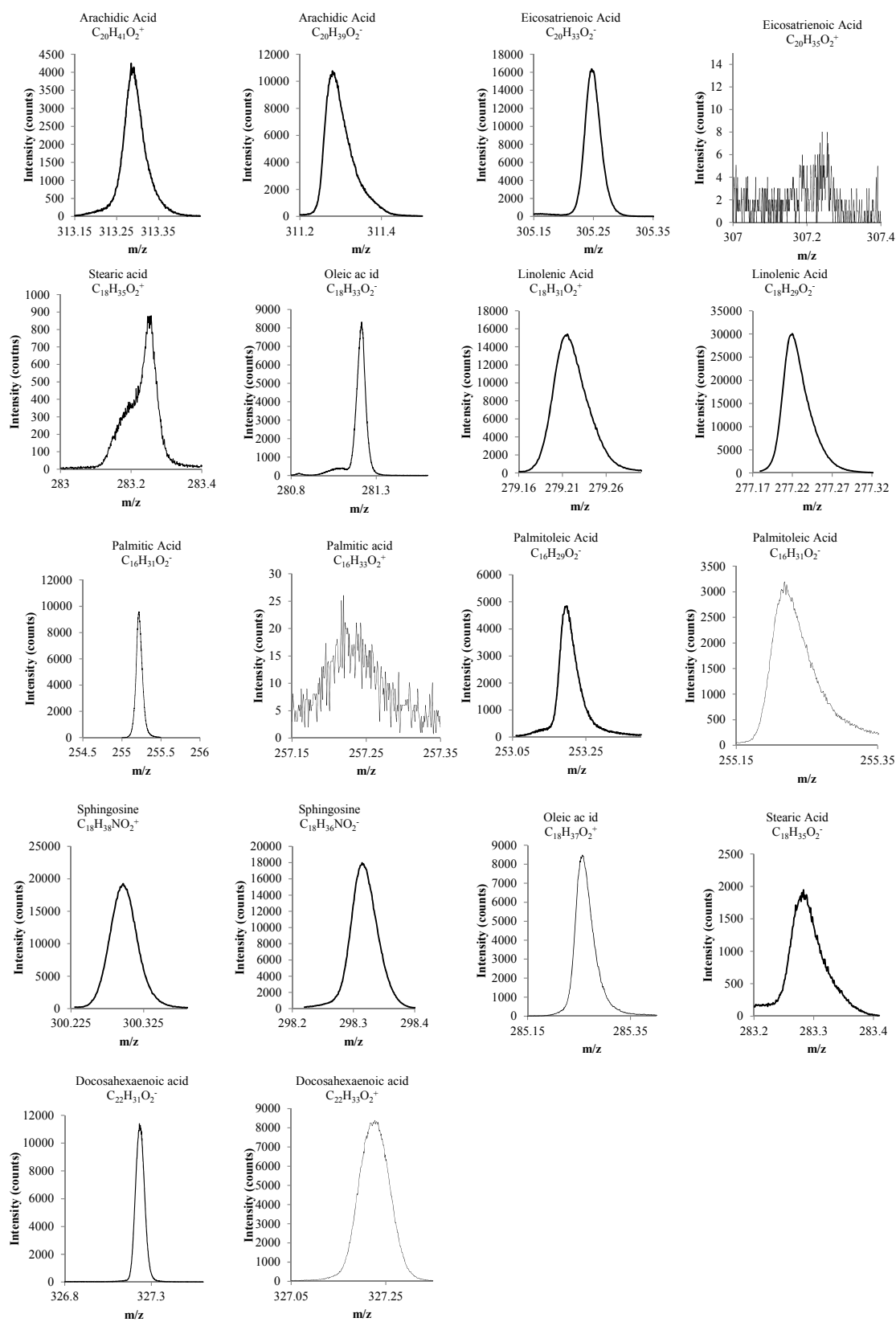
Accession #

01495-04, 01495-05, 01495-06

■ Host Material:	Silicon wafer
■ Technique:	SIMS
Analyzer Type:	time-of-flight
Secondary Source Polarity:	negative
Instrument:	ION-TOF, TOF.SIMS 5
Mass Range Minimum:	0 Da
Mass Range Maximum:	800 Da
Species Used for Mass Calibration:	CH ⁺ , OH ⁺ , C ₅ H ⁺
Analyzer Mass Resolution:	6021 m/Δm
Mass Resolution Determined at:	61 Da
Spectrum Dead Time Corrected?	No
Total Spectral Acquisition Time:	164 s
Abscissa Increment:	128 ps
Primary Beam Ion Gun:	LMIG
Primary Species:	Bi ₃ ⁺
Primary Ion Dose:	6.14 x 10 ¹⁰ ion/cm ²
Primary Ion Pulse Width:	17 ns
Primary Ion Pulse Rate:	10 kHz
Net Beam Voltage:	25000 eV
Pulsed Beam Current:	0.0004 nA
DC Beam Current:	Not specified

Beam Diameter:	1 μm
Beam Raster Size:	500 μm \times 500 μm
Specimen Normal-to-Analyzer:	Not specified
Beam Incident Angle:	45 $^\circ$
Source-to-Analyzer Angle:	45 $^\circ$
Comment:	Enter comment.

Figure 1 - EXPANDED [M+H]⁺ AND [M-H]⁻ PEAKS FOR EACH FATTY ACID SPECTRUM



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Accession # 01488-01, 01488-04, 01489-04, 01489-01, 01495-01, 01490-04, 01491-01, 01491-04, 01492-04, 01492-01, 01493-04, 01493-01, 01494-01, 01494-04, 01490-01, 01495-04, 01496-04, 01496-01

SPECTRAL FEATURES TABLE

Mass (Da)	Peak assignment	Positive polarity peaks present in following fatty acids	Peak most prominent in
27.023	C ₂ H ₃ ⁺	All fatty acids	
29.039	C ₂ H ₅ ⁺	All fatty acids	
39.023	C ₃ H ₃ ⁺	All fatty acids	
41.039	C ₃ H ₅ ⁺	All fatty acids	
43.055	C ₃ H ₇ ⁺	All fatty acids	
55.055	C ₄ H ₇ ⁺	All fatty acids	
57.070	C ₄ H ₉ ⁺	All fatty acids	
60.045	C ₂ H ₆ NO ⁺	Sphingosine	Sphingosine
67.055	C ₅ H ₇ ⁺	All fatty acids	
69.070	C ₅ H ₉ ⁺	All fatty acids	
79.055	C ₆ H ₇ ⁺	All fatty acids	
81.070	C ₆ H ₉ ⁺	All fatty acids	
82.066	C ₅ H ₈ N ⁺	Sphingosine	Sphingosine
83.086	C ₆ H ₁₁ ⁺	All fatty acids	
91.055	C ₇ H ₇ ⁺	All fatty acids	
93.070	C ₇ H ₉ ⁺	All fatty acids	
95.086	C ₇ H ₁₁ ⁺	All fatty acids	
97.102	C ₇ H ₁₃ ⁺	All fatty acids	
105.070	C ₈ H ₉ ⁺	All fatty acids	
107.086	C ₈ H ₁₁ ⁺	All fatty acids	
109.102	C ₈ H ₁₃ ⁺	All fatty acids	
111.081	C ₇ H ₁₁ O ⁺	Multiple fatty acids	Stearic Acid
112.089	C ₇ H ₁₂ O ⁺	Multiple fatty acids	Arachidic Acid, Sphingosine, Stearic Acid
115.055	C ₉ H ₇ ⁺	Multiple fatty acids	Linolenic Acid
125.097	C ₈ H ₁₃ O ⁺	Multiple fatty acids	Stearic Acid
129.092	C ₇ H ₁₃ O ₂ ⁺	Arachidic Acid, Palmitoleic Acid, Stearic Acid	Stearic Acid
138.104	C ₉ H ₁₄ O ⁺	Sphingosine	Sphingosine
139.112	C ₉ H ₁₅ O ⁺	Multiple fatty acids	Stearic Acid
143.107	C ₈ H ₁₅ O ₂ ⁺	Multiple fatty acids	Stearic Acid
147.081	C ₁₀ H ₁₁ O ⁺	Multiple fatty acids	Eicosatrienoic Acid, Linolenic Acid, Palmitic Acid
153.128	C ₁₀ H ₁₇ O ⁺	Multiple fatty acids	Stearic Acid
155.107	C ₉ H ₁₅ O ₂ ⁺	Multiple fatty acids	Palmitoleic Acid
157.123	C ₉ H ₁₇ O ₂ ⁺	Arachidic Acid, Palmitoleic Acid, Stearic Acid	Stearic Acid
165.128	C ₁₁ H ₁₇ O ⁺	Palmitoleic Acid	Palmitoleic Acid
167.144	C ₁₁ H ₁₉ O ⁺	Stearic Acid	Stearic Acid
171.081	C ₁₂ H ₁₁ O ⁺	Eicosatrienoic Acid	
171.117	C ₁₃ H ₁₅ ⁺	Linolenic Acid	Linolenic Acid
171.138	C ₁₀ H ₁₉ O ₂ ⁺	Stearic Acid	Stearic Acid
173.060	C ₁₁ H ₉ O ₂ ⁺	Sphingosine	Sphingosine
178.042	C ₁₃ H ₆ O ⁺	Arachidic Acid, Sphingosine, Stearic Acid	Arachidic Acid
181.123	C ₁₁ H ₁₇ O ₂ ⁺	Multiple fatty acids	Linolenic Acid, Palmitoleic Acid
185.154	C ₁₁ H ₂₁ O ₂ ⁺	Arachidic Acid, Stearic Acid	Stearic Acid
195.138	C ₁₂ H ₁₉ O ₂ ⁺	Eicosatrienoic Acid, , Linolenic Acid	Linolenic Acid
195.175	C ₁₃ H ₂₃ O ⁺	Stearic Acid	Stearic Acid
196.146	C ₁₂ H ₂₀ O ₂ ⁺	Multiple fatty acids	Linolenic Acid, Palmitoleic Acid, Sphingosine
209.154	C ₁₃ H ₂₁ O ₂ ⁺	Linolenic Acid, Palmitoleic Acid	Linolenic Acid
209.191	C ₁₄ H ₂₅ O ⁺	Stearic Acid	Stearic Acid
210.162	C ₁₃ H ₂₂ O ₂ ⁺	Sphingosine	Linolenic Acid, Palmitoleic Acid, Sphingosine
221.154	C ₁₄ H ₂₁ O ₂ ⁺	Multiple fatty acids	Eicosatrienoic Acid
221.191	C ₁₅ H ₂₅ O ⁺	Linolenic Acid	Linolenic Acid
222.162	C ₁₄ H ₂₂ O ₂ ⁺	Linolenic Acid	Linolenic Acid
223.170	C ₁₄ H ₂₃ O ₂ ⁺	Linolenic Acid	Linolenic Acid
223.206	C ₁₅ H ₂₇ O ⁺	Arachidic Acid, Stearic Acid	Arachidic Acid
224.178	C ₁₄ H ₂₄ O ₂ ⁺	Linolenic Acid, Sphingosine	Sphingosine

237.185	C ₁₅ H ₂₅ O ₂ ⁺	Linolenic Acid	Linolenic Acid
237.222	C ₁₆ H ₂₉ O ⁺	Multiple fatty acids	Palmitic Acid, Palmitoleic Acid
238.193	C ₁₅ H ₂₆ O ₂ ⁺	Sphingosine	Sphingosine
239.237	C ₁₆ H ₃₁ O ⁺	Stearic Acid	Stearic Acid
251.201	C ₁₆ H ₂₇ O ₂ ⁺	Palmitoleic Acid	Palmitoleic Acid
251.237	C ₁₇ H ₃₁ O ⁺	Arachidic Acid, Sphingosine, Stearic Acid	Arachidic Acid
252.209	C ₁₆ H ₂₈ O ₂ ⁺	Palmitic Acid, Palmitoleic Acid	Palmitic Acid, Palmitoleic Acid
253.217	C ₁₆ H ₂₉ O ₂ ⁺	Palmitic Acid, Palmitoleic Acid, Stearic Acid	Palmitic Acid, Palmitoleic Acid
254.225	C ₁₆ H ₃₀ O ₂ ⁺	Palmitic Acid, Palmitoleic Acid, Sphingosine	Palmitoleic Acid
255.232	C ₁₆ H ₃₁ O ₂ ⁺	Palmitic Acid, Palmitoleic Acid	Palmitic Acid, Palmitoleic Acid
256.240	C ₁₆ H ₃₂ O ₂ ⁺	Palmitic Acid, Palmitoleic Acid	Palmitic Acid
257.248	C ₁₆ H ₃₃ O ₂ ⁺	Palmitic Acid, Stearic Acid	Stearic Acid
261.222	C ₁₈ H ₂₉ O ⁺	Linolenic Acid, Palmitoleic Acid	Linolenic Acid
263.237	C ₁₈ H ₃₁ O ⁺	Eicosatrienoic Acid	Eicosatrienoic Acid
265.253	C ₁₈ H ₃₃ O ⁺	Oleic Acid, Arachidic Acid	Oleic Acid, Arachidic Acid
267.269	C ₁₈ H ₃₅ O ⁺	Arachidic Acid	Arachidic Acid
277.217	C ₁₈ H ₂₉ O ₂ ⁺	Multiple fatty acids	Linolenic Acid, Palmitic Acid, Palmitoleic Acid
278.225	C ₁₈ H ₃₀ O ₂ ⁺	Multiple fatty acids	Linolenic Acid
279.232	C ₁₈ H ₃₁ O ₂ ⁺	Eicosatrienoic Acid, Linolenic Acid	Eicosatrienoic Acid, Linolenic Acid
280.240	C ₁₈ H ₃₂ O ₂ ⁺	Multiple fatty acids	Eicosatrienoic Acid
281.191	C ₂₀ H ₂₅ O ⁺	Oleic Acid, Arachidic Acid	Oleic Acid, Arachidic Acid
282.256	C ₁₈ H ₃₄ O ₂ ⁺	Sphingosine	Sphingosine
283.264	C ₁₈ H ₃₅ O ₂	Oleic Acid	Oleic Acid
285.279	C ₁₈ H ₃₇ O ₂ ⁺	Stearic Acid	Stearic Acid
293.284	C ₂₀ H ₃₇ O ⁺	Arachidic Acid	Arachidic Acid
295.300	C ₂₀ H ₃₉ O ⁺	Arachidic Acid	Arachidic Acid
296.308	C ₂₀ H ₄₀ O ⁺	Arachidic Acid	Arachidic Acid
300.290	C ₁₈ H ₃₈ NO ₂ ⁺	Sphingosine	Sphingosine
311.295	C ₂₀ H ₃₉ O ₂ ⁺	Arachidic Acid	Arachidic Acid
312.303	C ₂₀ H ₄₀ O ₂ ⁺	Arachidic Acid	Arachidic Acid
313.311	C ₂₀ H ₄₁ O ₂ ⁺	Arachidic Acid	Arachidic Acid
322.275	C ₂₀ H ₃₆ NO ₂ ⁺	Sphingosine	Sphingosine
327.232	C ₂₂ H ₃₁ O ₂ ⁺	Docosahexaenoic acid	Docosahexaenoic acid
329.247	C ₂₂ H ₃₃ O ₂ ⁺	Docosahexaenoic acid	Docosahexaenoic acid
327.231	C ₂₂ H ₃₁ O ₂ ⁺	Docosahexaenoic acid	Docosahexaenoic acid

SPECTRAL FEATURES TABLE

Mass (Da)	Peak assignment	Negative polarity peaks present in following fatty acids	Peak most prominent in
25.010	C ₂ H ⁺	All fatty acids	
26.003	CN ⁺	Sphingosine	Sphingosine
41.003	C ₂ HO ⁻	All fatty acids	
44.998	CHO ₂ ⁻	Multiple fatty acids	Arachidic Acid, Eicosatrienoic Acid, Linolenic Acid, Sphingosine
49.008	C ₄ H ⁺	All fatty acids	
58.005	C ₂ H ₂ O ₂ ⁻	All fatty acids	
58.029	C ₂ H ₄ NO ⁻	Sphingosine	Sphingosine
71.013	C ₃ H ₃ O ₂ ⁻	All fatty acids	
85.029	C ₄ H ₅ O ₂ ⁻	All fatty acids	
93.034	C ₆ H ₅ O ⁻	Sphingosine	Sphingosine
95.050	C ₆ H ₇ O ⁻	Sphingosine	Sphingosine
99.045	C ₅ H ₇ O ₂ ⁻	All fatty acids	
113.060	C ₆ H ₉ O ₂ ⁻	All fatty acids	
127.076	C ₇ H ₁₁ O ₂ ⁻	All fatty acids	
141.092	C ₈ H ₁₃ O ₂ ⁻	All fatty acids	
155.107	C ₉ H ₁₅ O ₂ ⁻	All fatty acids	
163.076	C ₁₀ H ₁₁ O ₂ ⁻	Eicosatrienoic Acid, Linolenic Acid	Eicosatrienoic Acid, Linolenic Acid
167.107	C ₁₀ H ₁₅ O ₂ ⁻	All fatty acids	
169.123	C ₁₀ H ₁₇ O ₂ ⁻	All fatty acids	
181.123	C ₁₁ H ₁₇ O ₂ ⁻	All fatty acids	
183.138	C ₁₁ H ₁₉ O ₂ ⁻	All fatty acids	
195.138	C ₁₂ H ₁₉ O ₂ ⁻	All fatty acids	
197.154	C ₁₂ H ₂₁ O ₂ ⁻	Arachidic Acid, Sphingosine, Stearic Acid	Arachidic Acid, Sphingosine, Stearic Acid
209.154	C ₁₃ H ₂₁ O ₂ ⁻	All fatty acids	
211.170	C ₁₃ H ₂₃ O ₂ ⁻	Arachidic Acid, Sphingosine, Stearic Acid	Arachidic Acid, Sphingosine, Stearic Acid
221.154	C ₁₄ H ₂₁ O ₂ ⁻	Multiple fatty acids	Eicosatrienoic Acid, Linolenic Acid, Stearic Acid
223.170	C ₁₄ H ₂₃ O ₂ ⁻	All fatty acids	Eicosatrienoic Acid, Linolenic Acid, Sphingosine Acid, Stearic Acid
225.185	C ₁₄ H ₂₅ O ₂ ⁻	Arachidic Acid, Sphingosine, Stearic Acid	Arachidic Acid, Sphingosine, Stearic Acid
227.201	C ₁₄ H ₂₇ O ₂ ⁻	Sphingosine, Stearic Acid	Sphingosine
235.170	C ₁₅ H ₂₃ O ₂ ⁻	Eicosatrienoic Acid, Linolenic Acid	Eicosatrienoic Acid, Linolenic Acid
237.185	C ₁₅ H ₂₅ O ₂ ⁻	Multiple fatty acids	Eicosatrienoic Acid, Linolenic Acid
237.222	C ₁₆ H ₂₉ O ⁻	Sphingosine	Sphingosine
239.201	C ₁₅ H ₂₇ O ₂ ⁻	Arachidic Acid, Stearic Acid	Arachidic Acid, Stearic Acid
249.185	C ₁₆ H ₂₅ O ₂ ⁻	Multiple fatty acids	Eicosatrienoic Acid, Linolenic Acid
251.201	C ₁₆ H ₂₇ O ₂ ⁻	Multiple fatty acids	Palmitic Acid, Palmitoleic Acid
252.209	C ₁₆ H ₂₈ O ₂ ⁻	Multiple fatty acids	Palmitic Acid, Palmitoleic Acid
253.217	C ₁₆ H ₂₉ O ₂ ⁻	Multiple fatty acids	Palmitic Acid, Palmitoleic Acid, Stearic Acid
253.253	C ₁₇ H ₃₃ O ⁻	Sphingosine	Sphingosine
254.225	C ₁₆ H ₃₀ O ₂ ⁻	Arachidic Acid, Palmitic Acid, Palmitoleic Acid	Palmitic Acid, Palmitoleic Acid
255.232	C ₁₆ H ₃₁ O ₂ ⁻	Arachidic Acid, Linolenic Acid, Stearic Acid	Linolenic Acid, Stearic Acid
263.201	C ₁₇ H ₂₇ O ₂ ⁻	Eicosatrienoic Acid, Linolenic Acid	Linolenic Acid
267.232	C ₁₇ H ₃₁ O ₂ ⁻	Arachidic Acid, Stearic Acid	Arachidic Acid, Stearic Acid
277.217	C ₁₈ H ₂₉ O ₂ ⁻	Oleic Acid, Eicosatrienoic Acid, Linolenic Acid	Oleic Acid, Eicosatrienoic Acid, Linolenic Acid
278.225	C ₁₈ H ₃₀ O ₂ ⁻	Eicosatrienoic Acid, Linolenic Acid	Linolenic Acid
279.232	C ₁₈ H ₃₁ O ₂ ⁻	Multiple fatty acids	Oleic Acid, Eicosatrienoic Acid, Linolenic Acid
280.240	C ₁₈ H ₃₂ O ₂ ⁻	Stearic Acid	Stearic Acid
281.248	C ₁₈ H ₃₃ O ₂ ⁻	Multiple fatty acids	Arachidic Acid, Stearic Acid
282.256	C ₁₈ H ₃₄ O ₂ ⁻	Stearic Acid	Stearic Acid
283.264	C ₁₈ H ₃₅ O ₂ ⁻	Stearic Acid	Stearic Acid
284.272	C ₁₈ H ₃₆ O ₂ ⁻	Stearic Acid	Stearic Acid
295.264	C ₁₉ H ₃₅ O ₂ ⁻	Arachidic Acid	Arachidic Acid
298.275	C ₁₈ H ₃₆ NO ₂ ⁻	Sphingosine	Sphingosine
305.248	C ₂₀ H ₃₃ O ₂ ⁻	Eicosatrienoic Acid	Eicosatrienoic Acid
311.295	C ₂₀ H ₃₉ O ₂ ⁻	Arachidic Acid	Arachidic Acid
327.231	C ₂₂ H ₃₁ O ₂ ⁻	Docosahexaenoic acid	Docosahexaenoic acid

